Access DB# 125479

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Allen Pryor Examiner #: 74458 Date: 6/23/04
Art Unit: 1616 Phone Number ~~30~~ 2-0621 Serial Number: 10/797,355
Mail Box and Bldg/Room Location: REM 4A39 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

****

STAFF USE ONLY	**Type of Search**		**Vendors and cost where applicable**
Searcher: Sheppard	NA Sequence (#)		STN
Searcher Phone #:	AA Sequence (#)		Dialog
Searcher Location:	Structure (#)		Questel/Orbit
Date Searcher Picked Up:	Bibliographic		Dr.Link
Date Completed: 6/23/04	Litigation		Lexis/Nexis
Searcher Prep & Review Time:	Fulltext		Sequence Systems
Clerical Prep Time:	Patent Family		WWW/Internet
Online Time:	Other		Other (specify)

PTO-1590 (8-01)

STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 125479

TO: Alton Pryor Location: REM 4A39 Art Unit: 1616 June 23, 2004 Case Serial Number: 10/797355	From: P. Sheppard Location: Remsen Building Phone: (571) 272-2529 sheppard@uspto.gov

4670

Search Notes

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FILE 'HCAPLUS' ENTERED AT 15:04:25 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 23 Jun 2004  VOL 140 ISS 26
FILE LAST UPDATED: 22 Jun 2004  (20040622/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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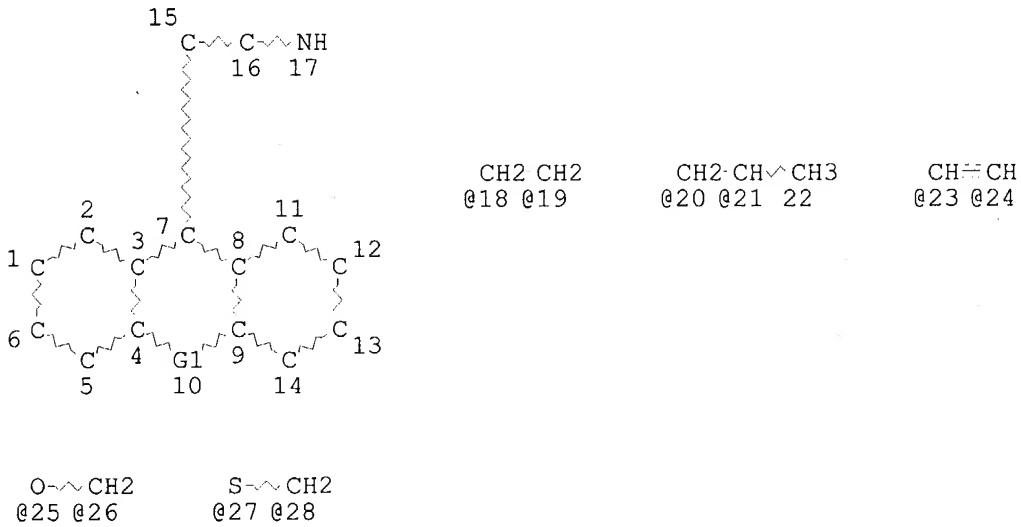


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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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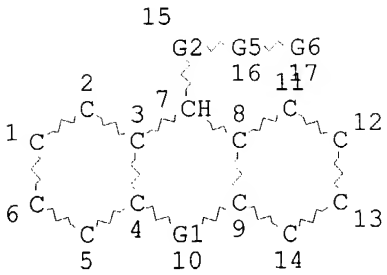

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE
L10 44 SEA FILE=REGISTRY SUB=L5 SSS FUL L9
L11 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L10

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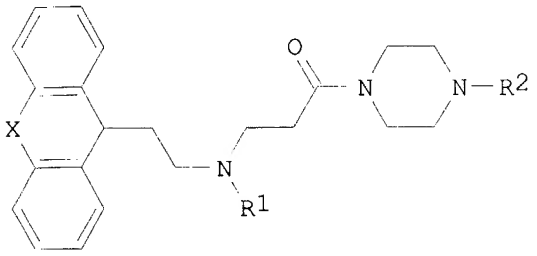
L11 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:376846 HCAPLUS
DOCUMENT NUMBER: 138:368918
TITLE: Preparation of piperazine derivatives having SST1 antagonistic activity
INVENTOR(S): Troxler, Thomas J.; Hoyer, Daniel
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma Gmbh
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040125	A1	20030515	WO 2002-EP12514	20021108

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR

PRIORITY APPLN. INFO.: GB 2001-27008 A 20011109
OTHER SOURCE(S): MARPAT 138:368918
GI

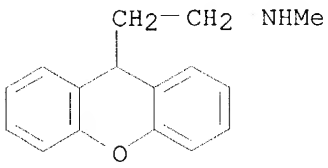


I

AB The title compds. [I; X = a bond, O, S, CH2, CH:CH, CH2CH2; R1 = alkyl, alkenyl, (cycloalkyl)alkyl; R2 = (un)substituted Ph, 2-oxopyridyl, pyridyl, etc.] and their pharmaceutically acceptable acid addition salts, useful for the treatment of depression, anxiety and bipolar disorders, were prepared E.g., a multi-step synthesis of I [X = O; R1 = Me; R2 = 3,4-F2C6H3], starting from 9H-xanthen-9-ol and malonic acid, was given. The latter has high affinity for somatostatin receptors, independently of the species, and is SST1 selective. Its pKd values are as follows 8.3-8.8, 8.0-8.4, and 9.1 in human, mouse, and rat, resp.

IT **55286-76-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperazine derivs. having SST1 antagonistic activity)

RN 55286-76-5 HCAPLUS
CN 9H-Xanthene-9-ethanamine, N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:866076 HCAPLUS
DOCUMENT NUMBER: 138:106626
TITLE: Diastereoselective Synthesis of 2-Aminoalkyl-3-sulfonyl-1,3-oxazolidines on Solid Support
AUTHOR(S): Conde-Frieboes, Kilian; Schjeltved, Rie K.; Breinholt, Jens
CORPORATE SOURCE: Discovery Chemistry, Novo Nordisk A/S, Malov, DK-2760, Den.
SOURCE: Journal of Organic Chemistry (2002), 67(25), 8952-8957
CODEN: JOCEAH; ISSN: 0022-3263

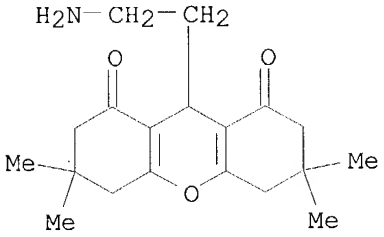
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:106626

AB Herein we report our investigation on the oxidation of solid-support-bound amino alcs. to aldehydes. These aldehydes were converted to diastereomerically pure (>10:1) 2,4-cis-2-aminoalkyl-3-sulfonyl-1,3-oxazolidines using optically pure 1,2-amino alcs. The relative configuration was determined using the nuclear Overhauser effect. The synthesized oxazolidines, which were obtained in high purities, represent a new, diverse scaffold for the solid-phase synthesis of libraries directed toward a pharmacol. target.

IT **488139-42-0P**
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(diastereoselective preparation of 2-(aminoalkyl)-3-sulfonyl-1,3-oxazolidines on solid support)

RN 488139-42-0 HCAPLUS

CN 1H-Xanthene-1,8(2H)-dione, 9-(2-aminoethyl)-3,4,5,6,7,9-hexahydro-3,3,6,6-tetramethyl- (9CI) (CA INDEX NAME)



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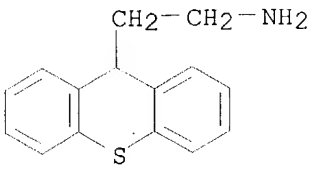
L11 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:830459 HCAPLUS
DOCUMENT NUMBER: 136:160841
TITLE: Structure-activity relationship studies on the potent multidrug resistance (MDR) modulator 2-(3,4-dimethoxyphenyl)-2-(methylethyl)-5-[(anthr-9-yl)methylamino]pentanenitrile (MM 36)
AUTHOR(S): Teodori, Elisabetta; Dei, Silvia; Garnier-Suillerot, Arlette; Quidu, Patricia; Scapecchi, Serena; Budriesi, Roberta
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita' di Firenze, Florence, 50121, Italy
SOURCE: Medicinal Chemistry Research (2001), 10(9), 563-576
CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser Boston
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A few derivs. of the potent MDR inhibitor 2-(3,4-dimethoxyphenyl)-2-(methylethyl)-5-[(anthr-9-yl)methylamino]pentanenitrile were synthesized and studied with the aim of optimizing activity and selectivity. Thus, even if dramatic improvements in potency and in selectivity were not reached, a better drug candidate and a new lead for further development of the series were identified.

IT **21745-81-3P**, 9H-Thioxanthene-9-ethanamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationship studies on potent multidrug resistance modulator 2-(3,4-dimethoxyphenyl)-2-(methylethyl)-5-[(anthr-9-

yl)methylamino]pentanenitrile)
RN 21745-81-3 HCAPLUS
CN 9H-Thioxanthene-9-ethanamine (9CI) (CA INDEX NAME)



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L11 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:66753 HCAPLUS
DOCUMENT NUMBER: 132:107773
TITLE: Preparation of aralkylamines as NMDA receptor-ionophore complex antagonists
INVENTOR(S): Mueller, Alan L.; Balandrin, Manuel F.; Vanwagenen, Bradford C.; Moe, Scott T.; Delmar, Eric G.; Artman, Linda D.; Barmore, Robert M.; Smith, Daryl L.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: U.S., 112 pp., Cont.-in-part of U.S. Ser. No. 663.013.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6017965	A	20000125	US 1996-763480	19961211
CA 2182680	AA	19950817	CA 1994-2182680	19941026
WO 9521612	A2	19950817	WO 1994-US12293	19941026
WO 9521612	A3	19950921		
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CN 1148337	A	19970423	CN 1994-195074	19941026
CN 1088585	B	20020807		
ES 2156162	T3	20010616	ES 1994-932057	19941026
EP 1123922	A2	20010816	EP 2000-121960	19941026
EP 1123922	A3	20040102		
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PT 743853	T	20011031	PT 1994-932057	19941026
US 6071970	A	20000606	US 1995-485038	19950607
CA 2257234	AA	19971211	CA 1996-2257234	19961211
US 6211245	B1	20010403	US 1998-186341	19981104
AU 770292	B2	20040219	AU 2000-71810	20001124
US 2002004522	A1	20020110	US 2001-825373	20010402
US 6750244	B2	20040615		
JP 2004002437	A2	20040108	JP 2003-158350	20030603

PRIORITY APPLN. INFO.:
US 1993-14813 B2 19930208
US 1994-194210 B2 19940208
US 1994-288668 B2 19940809
WO 1994-US12293 A2 19941026

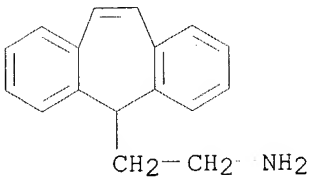
US	1995-485038	A2 19950607
US	1996-663013	A2 19960607
US	1994-288688	A2 19940811
EP	1994-932057	A3 19941026
JP	1995-521191	A3 19941026
WO	1996-US19525	A 19961206
AU	1997-13525	A3 19961211
US	1996-763480	A2 19961211
US	1997-869154	B2 19970604
US	1997-873011	A1 19970611
US	1998-186341	A1 19981104

OTHER SOURCE(S): MARPAT 132:107773

AB R7CHR4CR1R5CRR2R6[I; R = H or N(R3)2; R1,R5 = (un)substituted Ph, -CH2Ph, -OPh; R2,R6 = H or (hydroxy)alkyl; R1R2 = (CH2)n or (CH2)nNR3(CH2)n; R2R6 = NH; R3 = H, alkyl, CH2CH2OH, alkylphenyl; R4 = (un)substituted Ph, -pyridyl, -thienyl, etc.; R7 = (un)substituted Ph; n = 0-6] were prepared Thus, (3-FC6H4)2CO was condensed with (EtO)2P(O)CH2CO2Et and the product converted in 6 steps to (3-FC6H4)2CHCH2CHMeNH2. Data for biol. activity of I were given.

IT **14451-09-3P**, 5H-Dibenzo[a,d]cycloheptene-5-ethanamine
21745-77-7P, 9H-Xanthene-9-ethanamine **21745-81-3P**,
9H-Thioxanthene-9-ethanamine **21745-82-4P 21745-83-5P**
21745-85-7P 200430-08-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aralkylamines as NMDA receptor-ionophore complex antagonists)

RN 14451-09-3 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine (9CI) (CA INDEX NAME)



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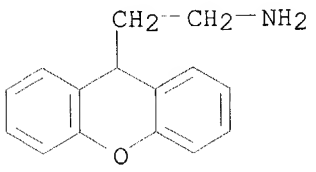

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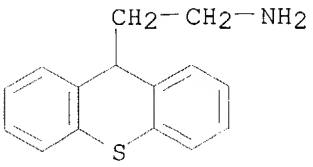

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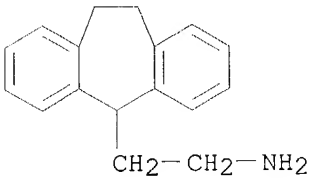
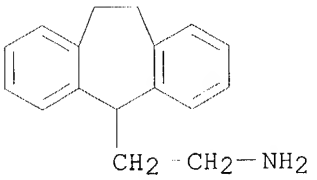
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro- (9CI) (CA INDEX NAME)

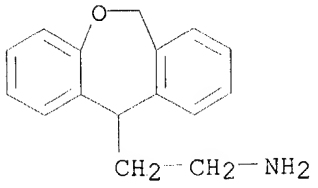


RN 21745-83-5 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)

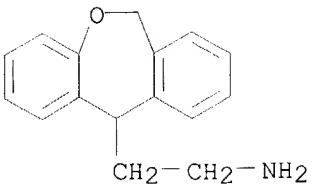


● HCl

RN 21745-85-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro- (9CI) (CA INDEX NAME)



RN 200430-08-6 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 172 THERE ARE 172 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:53380 HCAPLUS
DOCUMENT NUMBER: 132:93096
TITLE: Preparation of diarylalkylamines and related compounds active at both the serotonin reuptake site and the N-methyl-D-aspartate receptor for treatment depression and other disorders.
INVENTOR(S): Mueller, Alan; Moe, Scott; Balandrin, Manuel
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000002551	A2	20000120	WO 1999-US15857	19990712
WO 2000002551	A3	20000921		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2336962	AA	20000120	CA 1999-2336962	19990712
AU 9949919	A1	20000201	AU 1999-49919	19990712
AU 771252	B2	20040318		
EP 1096926	A2	20010509	EP 1999-933987	19990712
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US 2004039014	A1	20040226	US 2001-990405	20011121

PRIORITY APPLN. INFO.: US 1998-92546P P 19980713
WO 1999-US15857 W 19990712

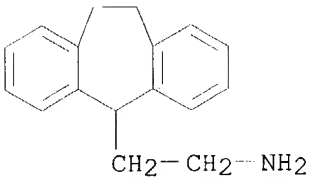
OTHER SOURCE(S): MARPAT 132:93096

AB A method for treatment of depression comprises administration of a compound having NMDA receptor binding activity of IC50 = 50 nM to 1 μM and serotonin reuptake IC50 ≤100 nM. The compds. include e.g. XmAr1(XmAr2)CHCR1R1CR2R2NR3R3 [X = Br, Cl, F, iodo, CF3, alkyl, OH, OCF3, alkoxy, acyloxy; Ar1, Ar2 = Ph, naphthyl, thiofuranyl, tetrahydronaphthyl, furyl, pyridyl, etc.; R1 = H, alkyl, hydroxyalkyl, OH, alkoxy, acyloxy; R2

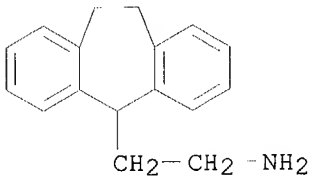
= H, alkyl, hydroxyalkyl; (R2)2 = imino; R3 = H, alkyl, HOCH2CH2, alkylphenyl; m = 0-5]. Thus, N-methyl-bis-[3-(3-fluorophenyl)]propylamine (preparation given) at 5 mg/kg orally in mice produced a time-dependent reduction in the duration of immobility in the forced swimming test.

IT **21745-82-4P 21745-83-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diarylalkylamines and related compds. active at both the serotonin reuptake site and the N-methyl-D-aspartate receptor for treatment depression and other disorders)

RN 21745-82-4 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro- (9CI) (CA INDEX NAME)



RN 21745-83-5 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L11 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:7958 HCAPLUS
DOCUMENT NUMBER: 130:66268
TITLE: Compounds active at a novel site on receptor-operated calcium channels useful for treatment of neurological disorders and diseases
INVENTOR(S): Mueller, Alan L.; Moe, Scott T.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 252 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9856752	A1	19981217	WO 1998-US11608	19980611
W: JP				

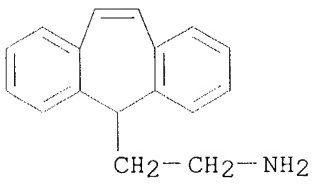
AU 770292 B2 20040219 AU 2000-71810 20001124
PRIORITY APPLN. INFO.: US 1997-873011 A 19970611
AU 1997-13525 A3 19961211
OTHER SOURCE(S): MARPAT 130:66268
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

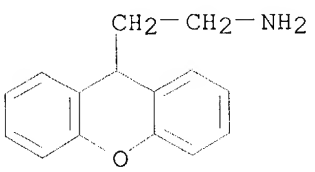
AB The compds. [I, II, III; R1 and R3 are independently selected from (un)substituted Ph, benzyl, phenoxy, H, alkyl, OH, etc.; R2 and R5 are independently selected from H, alkyl, hydroxyalkyl; R2-R5 together are imino; R1-R2 together are (CH2)n, (CH2)n-N(R6)-(CH2)n; n = 0-6, at least one n greater than 0; R6 is H, alkyl, 2-hydroxyethyl, and alkylphenyl; R4 is selected from (un)substituted thiofuryl, pyridyl, Ph, benzyl, phenoxy, phenylthio, H, alkyl, chcloalkyl; X, X1 is independently selected from (un)substituted Ph, benzyl, phenoxy, F, Cl, Br, Oh, etc.; m = 0-5; Y is N(R6)2, H when R1-R2 together are (CH2)n-N(R6)-(CH2)n], pharmaceutical compns., and pharmaceutical acceptable salts, complexes, and carriers are prepared as antagonists of NMDA receptor-mediated responses for treating a neurol. disease or disorder such as stroke, head trauma, spinal cord injury, spinal cord ischemia, ischemia- or hypoxia-induced nerve cell damage, epilepsy, anxiety, neuropsychiatric or cognitive deficits due to ischemia or hypoxia such as those that frequently occur as a consequence of cardiac surgery under cardiopulmonary bypass, or neurodegenerative diseases such as Alzheimer's Disease, Huntington's Disease, Parkinson's Disease, or amyotrophic lateral sclerosis (ALS).

IT **14451-09-3P**, 5H-Dibenzo[a,d]cycloheptene-5-ethanamine
21745-77-7P, 9H-Xanthene-9-ethanamine **21745-81-3P**,
9H-Thioxanthene-9-ethanamine **21745-82-4P 200429-81-8P**
200429-82-9P 200429-84-1P 200430-08-6P
217661-22-8P 217661-23-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(compds. active at novel site on receptor-operated calcium channels useful for treatment of neurol. disorders and diseases)

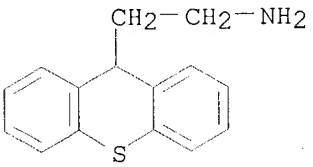
RN 14451-09-3 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine (9CI) (CA INDEX NAME)



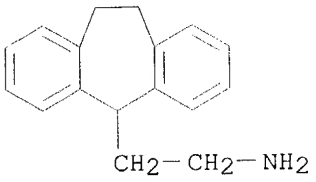
RN 21745-77-7 HCAPLUS
CN 9H-Xanthene-9-ethanamine (9CI) (CA INDEX NAME)



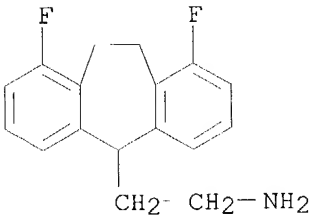
RN 21745-81-3 HCAPLUS
CN 9H-Thioxanthene-9-ethanamine (9CI) (CA INDEX NAME)



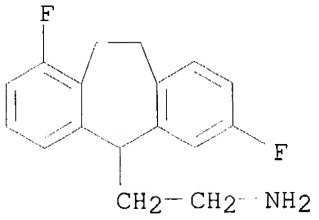
RN 21745-82-4 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro- (9CI) (CA INDEX NAME)



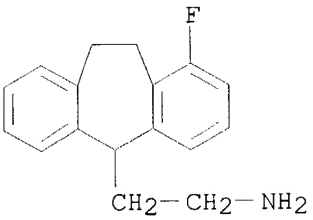
RN 200429-81-8 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1,9-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



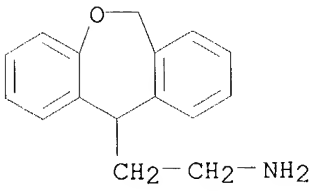
RN 200429-82-9 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1,7-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



RN 200429-84-1 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)

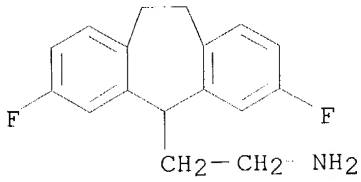


RN 200430-08-6 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)



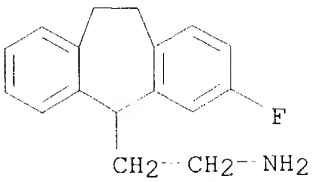
● HCl

RN 217661-22-8 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3,7-difluoro-10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 217661-23-9 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-fluoro-10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:1444 HCAPLUS
DOCUMENT NUMBER: 128:61341
TITLE: Preparation of aralkylamines as NMDA receptor-ionophore complex antagonists
INVENTOR(S): Mueller, Alan L.; Moe, Scott T.; Balandrin, Manuel F.; Vanwagenen, Bradford C.; Delmar, Eric G.; Artman, Linda D.; Barmore, Robert M.; Smith, Daryl L.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 298 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9746511	A1	19971211	WO 1996-US20697	19961211
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2257234	AA	19971211	CA 1996-2257234	19961211
AU 9713525	A1	19980105	AU 1997-13525	19961211
AU 723349	B2	20000824		
EP 912494	A1	19990506	EP 1996-945069	19961211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002511835	T2	20020416	JP 1998-500538	19961211
AU 770292	B2	20040219	AU 2000-71810	20001124

PRIORITY APPLN. INFO.:
US 1996-663013 A 19960607
WO 1996-US19525 A 19961206
AU 1997-13525 A3 19961211
WO 1996-US20697 W 19961211

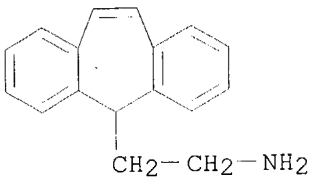
OTHER SOURCE(S): MARPAT 128:61341

AB R7CHR4CR1R5CRR2R6 [I; R = H or N(R3)2; R1,R5 = (un)substituted Ph, -CH2Ph, -OPh; R2,R6 = H or (hydroxy)alkyl; R1R2 = (CH2)n or (CH2)nNR3(CH2)n; R2R6 = NH; R3 = H, alkyl, CH2CH2OH, alkylphenyl; R4 = (un)substituted Ph, -pyridyl, -thienyl, etc.; R7 = (un)substituted Ph; n = 0-6] were prepared Thus, (3-FC6H4)2CO was condensed with (EtO)2P(O)CH2CO2Et and the product converted in 6 steps to (3-FC6H4)2CHCH2CHMeNH2. Data for biol. activity of I were given.

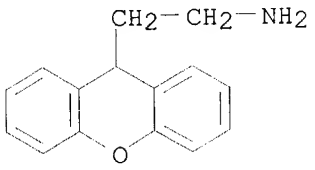
IT **14451-09-3P**, 5H-Dibenzo[a,d]cycloheptene-5-ethanamine
21745-77-7P, 9H-Xanthene-9-ethanamine **21745-81-3P**,

9H-Thioxanthene-9-ethanamine **21745-82-4P 21745-83-5P**
21745-85-7P 200429-81-8P 200429-82-9P
200429-83-0P 200429-84-1P 200429-85-2P
200430-08-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aralkylamines as NMDA receptor-ionophore complex antagonists)

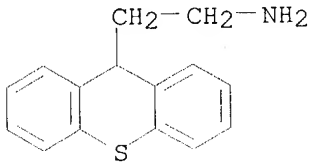
RN 14451-09-3 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine (9CI) (CA INDEX NAME)



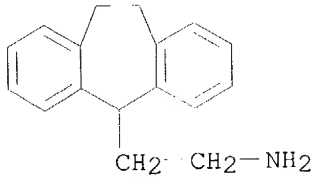
RN 21745-77-7 HCAPLUS
CN 9H-Xanthene-9-ethanamine (9CI) (CA INDEX NAME)



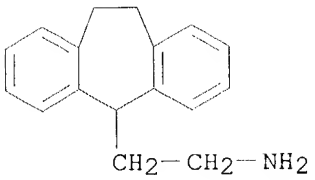
RN 21745-81-3 HCAPLUS
CN 9H-Thioxanthene-9-ethanamine (9CI) (CA INDEX NAME)



RN 21745-82-4 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro- (9CI) (CA INDEX NAME)

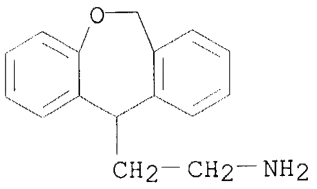


RN 21745-83-5 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)

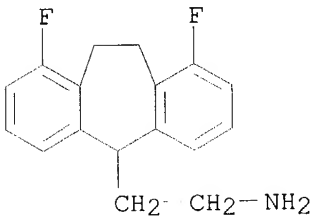


● HCl

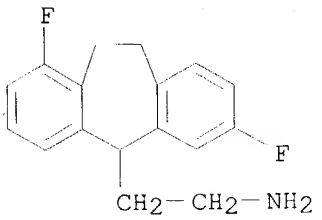
RN 21745-85-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro- (9CI) (CA INDEX NAME)



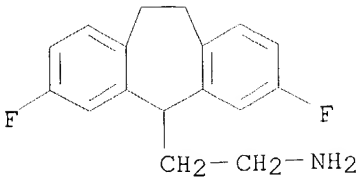
RN 200429-81-8 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1,9-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



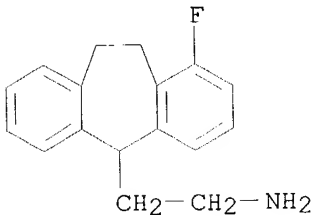
RN 200429-82-9 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1,7-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



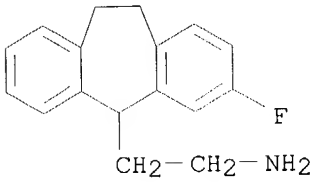
RN 200429-83-0 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3,7-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



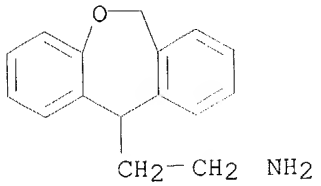
RN 200429-84-1 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



RN 200429-85-2 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)



RN 200430-08-6 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)



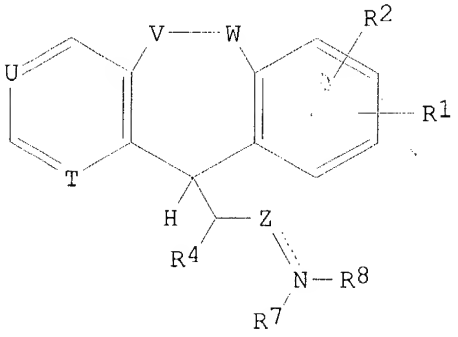
● HCl

L11 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:943447 HCAPLUS
DOCUMENT NUMBER: 123:339772
TITLE: Preparation of tricyclic tumor necrosis factor-α inhibitors
INVENTOR(S): Ting, Pauline C.; Friary, Richard J.; Tom, Wing C.;

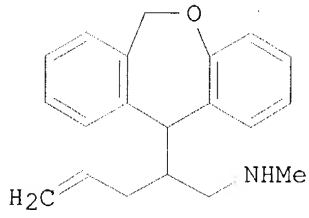
Lee, Joe F.; Seidl, Vera A.
PATENT ASSIGNEE(S): Schering Corp., USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9515959	A1	19950615	WO 1994-US13661	19941205
W: JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5574173	A	19961112	US 1993-162686	19931206
EP 733049	A1	19960925	EP 1995-903169	19941205
EP 733049	B1	19990310		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09500655	T2	19970121	JP 1994-516222	19941205
JP 2793914	B2	19980903		
AT 177425	E	19990315	AT 1995-903169	19941205
ES 2128701	T3	19990516	ES 1995-903169	19941205
CA 2175313	AA	19971030	CA 1996-2175313	19960429

PRIORITY APPLN. INFO.: US 1993-162686 19931206
WO 1994-US13661 19941205
OTHER SOURCE(S): MARPAT 123:339772
GI



I



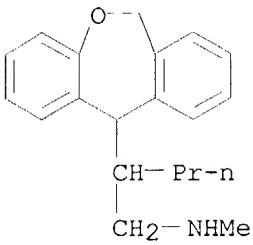
III

AB The title compds. [I; R1, R2 = H, halogen; R4 = alkenyl, alkoxy, OH; R7, R8 = H, alkyl, alkenyl, (un)substituted aryl, cycloalkyl, etc.; 1 of T and U is N and the other is :CH or both are :CH; 1 of V and W is O and the other is CH2 or both are CH2; Z = :CH, CH2, CH:CH, etc.; the dotted line is an optional double bond; NR7R8 = (un)substituted heterocyclyl], useful as tumor necrosis factor-α (II) inhibitors for treating septic shock, inflammation, or allergic diseases, are prepared and I-containing formulations presented. Thus, dibenzooxepine III was prepared and

demonstrated 54% II inhibition at 10 μM.

IT **170727-75-0P 170727-90-9P 170727-99-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tricyclic tumor necrosis factor-α inhibitors)

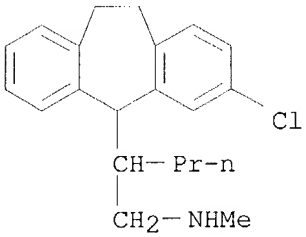
RN 170727-75-0 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl-β-propyl- (9CI) (CA INDEX NAME)



RN 170727-90-9 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-chloro-10,11-dihydro-N-methyl-β-propyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

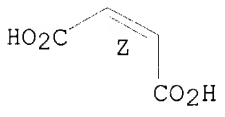
CRN 170727-89-6
CMF C21 H26 Cl N



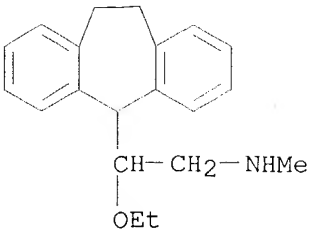
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



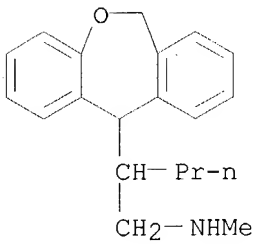
RN 170727-99-8 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, β-ethoxy-10,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)



IT **170727-82-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tricyclic tumor necrosis factor-α inhibitors)
RN 170727-82-9 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl-β-propyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

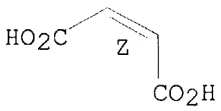
CRN 170727-75-0
CMF C20 H25 N O



CM 2

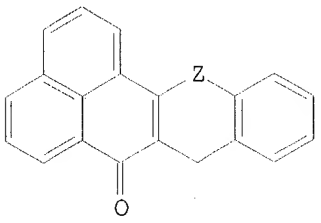
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

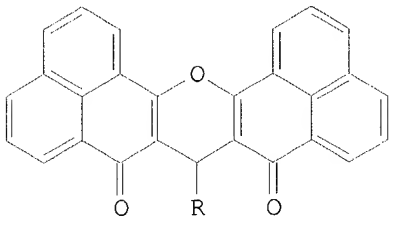


L11 ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:6529 HCAPLUS
DOCUMENT NUMBER: 96:6529
TITLE: Phenalenones. IV (1). Heterocycles from 3-hydroxyphenalenone (I)
AUTHOR(S): Kuroki, Masatane; Terachi, Yasuhito; Tsunashima, Yutaka
CORPORATE SOURCE: Dep. Chem., Shibaura Inst. Technol., Ohmiya, 330, Japan
SOURCE: Journal of Heterocyclic Chemistry (1981), 18(5), 873-6
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 96:6529
GI



I



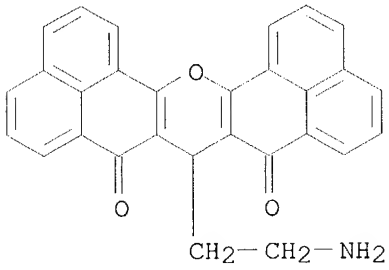
II

AB 3-Hydroxyphenalenone reacts with o-disubstituted benzenes (substituents: NH2, OH, CH2OH and SH), aliphatic and aromatic aldehydes to give various heterocyclic compds., e.g., I (Z = O, NH) and II (R = H, Me, aryl). These reactions resemble those of 1,3-cyclohexanediones in many respects.

IT **80090-01-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 80090-01-3 HCAPLUS

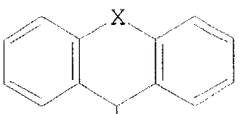
CN 7H,8H,9H-Dinaphtho[1,8-bc:1',8'-hi]xanthene-7,9-dione, 8-(2-aminoethyl)- (9CI) (CA INDEX NAME)



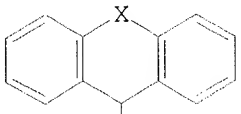
L11 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:16562 HCAPLUS
DOCUMENT NUMBER: 86:16562
TITLE: Amino alcohols with a tricyclic substituent
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H., Fed. Rep. Ger.
SOURCE: Fr. Demande, 13 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2277589	A1	19760206	FR 1974-24202	19740711
FR 2277589	B1	19781229		

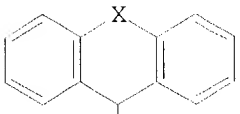
PRIORITY APPLN. INFO.: FR 1974-24202 19740711
GI



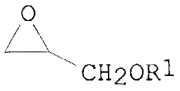
I



II



III



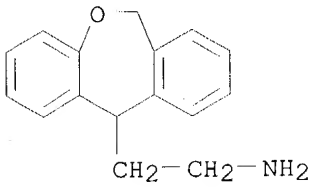
IV

AB Aminopropanediols I (X = CH2O, X1 = CH2, CH2CH2, CHMe, R = Me, R1 = Ph; X = O, S, CH2CH2, CH:CH, X1 = CH2, R = Me, R1 = Ph; X = CH2CH2, X1 = CMe2, R = Et, R1 = Ph; X = X1 = CH2CH2, R = Me, R1 = Ph; X = CH2O, X1 = CH2, R = Et, R1 = Ph; X = CH2O, X1 = CH2, R = Me, R1 = cyclohexyl) were prepared by treating mesylates II with MeNHCH2CH(OH)CH2OPh or by treating the amines III with the glycidyl ethers IV. I at 0.5 mg/kg orally in dogs increased heart output by 20-67% over controls.

IT **21745-85-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of)

RN 21745-85-7 HCAPLUS

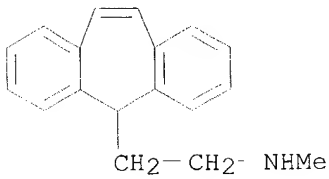
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro- (9CI) (CA INDEX NAME)



IT **7186-44-9P 55286-76-5P 55286-77-6P**
55286-79-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phenyl glycidyl ether)

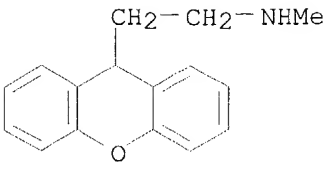
RN 7186-44-9 HCAPLUS

CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, N-methyl- (9CI) (CA INDEX NAME)

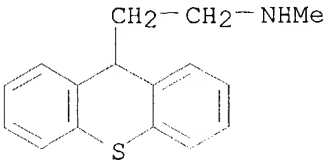


RN 55286-76-5 HCAPLUS

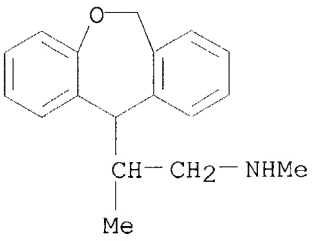
CN 9H-Xanthene-9-ethanamine, N-methyl- (9CI) (CA INDEX NAME)



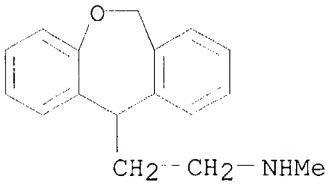
RN 55286-77-6 HCAPLUS
CN 9H-Thioxanthene-9-ethanamine, N-methyl- (9CI) (CA INDEX NAME)



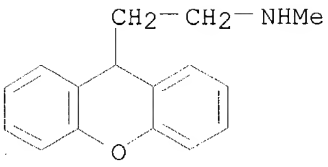
RN 55286-79-8 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N,β-dimethyl- (9CI) (CA INDEX NAME)



IT **55286-60-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phenylglycidyl ether)
RN 55286-60-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)

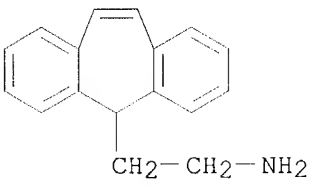


IT **61257-18-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61257-18-9 HCAPLUS
CN 9H-Xanthene-9-ethanamine, N-methyl-, hydrochloride (9CI) (CA INDEX NAME)

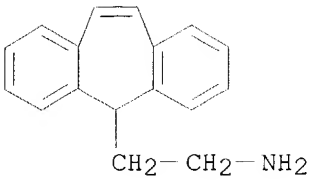


● HCl

L11 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:546868 HCAPLUS
DOCUMENT NUMBER: 83:146868
TITLE: Carbonium ion reactions. XII. Acetolysis of 5-(2-bromoethyl)-5H-dibenzo[a,d]cycloheptene and nitrous acid deamination of 5-(2-aminoethyl)-5H-dibenzo[a,d]cycloheptene
AUTHOR(S): Banciu, M.; Badea, F.; Jelescu, Rodica; Cioranescu, Ecaterina
CORPORATE SOURCE: Lab. Org. Chem., Polytech. Inst., Bucharest, Rom.
SOURCE: Revue Roumaine de Chimie (1975), 20(1), 121-7
CODEN: RRCHAX; ISSN: 0035-3930
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The products formed in the acetolysis of I (R = Br) (II) and in the deamination of I (R = NH2) (III) were similar to those obtained in the acetolysis of I (R = p-MeC6H4SO3) (IV). The rearranged cycloheptene double bond in I increased from 37 to 87 to 100% in the series III < IV < II; the importance of this route increased with the decreasing efficiency of the leaving group. The kinetics of the acetolysis were discussed.
IT **14451-09-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(deamination of, mechanism of)
RN 14451-09-3 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine (9CI) (CA INDEX NAME)



IT **21745-84-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21745-84-6 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, hydrochloride (9CI) (CA INDEX NAME)



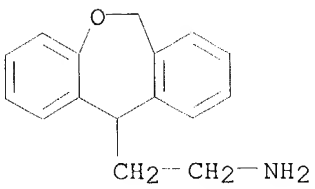
● HCl

L11 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:156136 HCAPLUS
DOCUMENT NUMBER: 82:156136
TITLE: 3-(Aryloxy)-2-hydroxypropylamine derivatives of tricyclic compounds as pharmaceuticals
INVENTOR(S): Winter, Werner; Thiel, Max; Stach, Kurt; Roesch, Egon; Sponer, Gisbert
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H.
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

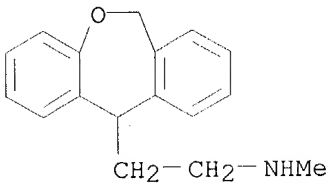
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2335943	A1	19750130	DE 1973-2335943	19730714
DE 2335943	C3	19790809		
DE 2335943	B2	19781207		
US 3944566	A	19760316	US 1974-484353	19740628
CA 1026325	A1	19780214	CA 1974-204154	19740705
ZA 7404363	A	19750827	ZA 1974-4363	19740708
FI 7402110	A	19750115	FI 1974-2110	19740709
FI 59588	B	19810529		
FI 59588	C	19810910		
GB 1410755	A	19751022	GB 1974-30356	19740709
AU 7471032	A1	19760115	AU 1974-71032	19740709
AT 7405671	A	19760415	AT 1974-5671	19740709
AT 333756	B	19761210		
CH 602579	A	19780731	CH 1974-9531	19740710
SE 7409183	A	19750115	SE 1974-9183	19740712
SE 410594	B	19791022		
NL 7409439	A	19750116	NL 1974-9439	19740712
NL 184004	B	19881017		
NL 184004	C	19890316		
JP 50037766	A2	19750408	JP 1974-81039	19740715
JP 59005577	B4	19840206		

PRIORITY APPLN. INFO.: DE 1973-2335943 19730714
GI For diagram(s), see printed CA Issue.
AB Hydroxypropylamines I (X = CH2O, O, S, CH2CH2, CH:CH, X1 = CH2CH2, R = Me, R1 = Ph; X = CH2O, CH2CH2, X1 = (CH2)3, R = Me, R1 = Ph; X = CH2O, X1 = CH2CH2, R = Et, R1 = Ph, R = Me, R1 = cyclohexyl; X = CH2O, X1 = CHMeCH2, R = Me, R1 = Ph; X = CH2CH2, X1 = CH2CMe2, R = Et, R1 = Ph), active on the heart and circulation, were prepared Thus, I (X = CH2O, X1 = CH2CH2, R = Me, R1 = Ph) was prepared by formylating 11-(2-aminoethyl)-6,11-dihydrodibenz[b,e]oxepin, reducing the formyl group, and treating the methylamine with phenyl glycidyl ether.

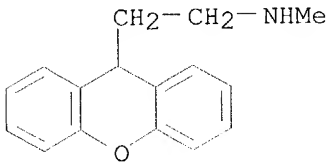
IT **21745-85-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of)
RN 21745-85-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro- (9CI) (CA INDEX NAME)



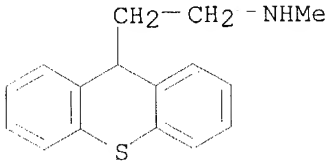
IT **55286-60-7P 55286-76-5P 55286-77-6P**
55286-79-8P 55286-80-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phenyl glycidyl ether)
RN 55286-60-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)



RN 55286-76-5 HCAPLUS
CN 9H-Xanthene-9-ethanamine, N-methyl- (9CI) (CA INDEX NAME)

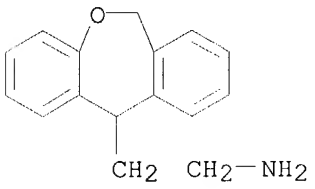


RN 55286-77-6 HCAPLUS
CN 9H-Thioxanthene-9-ethanamine, N-methyl- (9CI) (CA INDEX NAME)

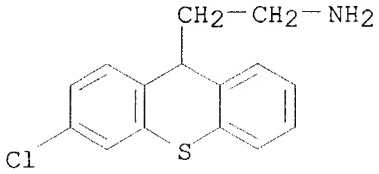


RN 55286-79-8 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N,β-dimethyl- (9CI) (CA INDEX NAME)

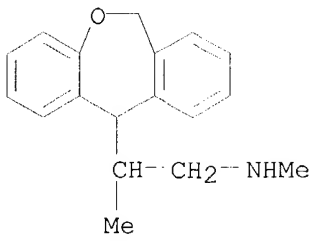
DE 1793735 C3 19750130
GB 1128938 A 19681002 GB 1967-33103 19670719
PRIORITY APPLN. INFO.: DE 1967-1793735 A 19670218
GI For diagram(s), see printed CA Issue.
AB Dibenzoxepinylethylamines I (X = O, R = cyclopentyl, cycloheptyl, cyclooctyl, cyclododecyl, 3-methylcyclohexyl, cyclohexylmethyl, 4-EtOC6H4, 3-MeC6H4, 3-O2N-C6H4CH2; X = S, R = 4-MeC6H4, 2-MeC6H4) were prepared in 54-81% yield by treating dibenzoxepinylethylamine with the epoxides II. II were prepared by treating epichlorohydrin with RXH. I enhance cardiac blood flow and are β-sympatholytics. Thus I (X = O, R = 4-EtOC6H4) at 0.5 mg/kg orally increased cardiac blood flow in dogs by 275%.
IT **21745-85-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with epoxy propanes)
RN 21745-85-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro- (9CI) (CA INDEX NAME)



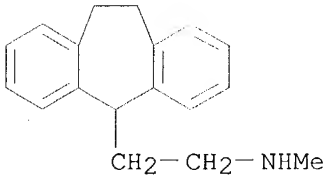
IT **53444-66-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with epoxypropane derivs.)
RN 53444-66-9 HCAPLUS
CN 9H-Thioxanthene-9-ethanamine, 3-chloro- (9CI) (CA INDEX NAME)



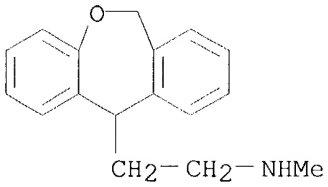
L11 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1970:100435 HCAPLUS
DOCUMENT NUMBER: 72:100435
TITLE: Synthesis of aminoalkylxanthenes and aminothioxanthenes
AUTHOR(S): Tsvetkova, I. D.; Orlova, E. K.; Zagorevskii, V. A.
CORPORATE SOURCE: Inst. Farmakol. Khimioter., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1969), 3(12), 17-20
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Derivs. of xanthene (I) and thioxanthene (II) were prepared Hydrogenation of Ia over Pd yielded 79.5% I [R = CH(CN)CO2Et] (III), m. 127-8°. Reduction of III with LiAlH4 gave 75% I [R = CH(CH2OH)CH2NH2] (IV), m. 115.5-16°; HCl salt m. 234-5°. Analogously, II [R = CH(CN)CO2Et] yielded 90% II [R = CH(CH2OH)CH2NH2] (V), m. 112.5-13°; HCl salt m. 215° (decomposition). A mixture of 0.5 g IV, 0.92 g HCO2H and 2 ml H2CO was boiled 7 hr and saturated with HCl to yield



RN 55286-80-1 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)



IT **55286-60-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyclohexyl glycidyl ether)
RN 55286-60-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)



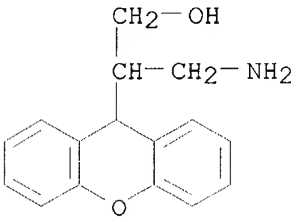
L11 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:505324 HCAPLUS
DOCUMENT NUMBER: 81:105324
TITLE: Tricyclic aminoalcohols and their nontoxic salts
INVENTOR(S): Winter, Werner; Thiel, Max; Stach, Kurt; Schaumann, Wolfgang; Dietmann, Karl
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H.
SOURCE: Ger., 6 pp. Division of Ger. 1,568,145 (See Brit. 1,128,938 CA 70;47324u).
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1793735	A1	19730726	DE 1967-1793735	19670218
DE 1793735	B2	19740606		

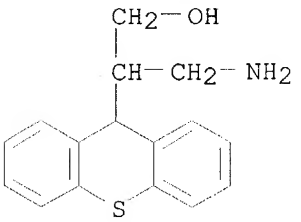
55% I [R = CH(CH2OH)CH2NMe2·HCl] (VI), 192° (decomposition). Treatment of VI with MeCOCl gave 96% I [R = CH(CH2O2CMe)CH2NMe2·HCl] (VII), m. 179-80° (decomposition). Boiling II [R = CH(CN)CO2Et] with C5H11N yielded 75% II [R = CH(CN)CONC5H10] (VIII), m. 190-1° (EtOH). Reduction of VIII with LiAlH4 gave 18% II [R = CH(CH2NC5H10)CH2NH2·2HCl] (IX), m. 250° (decomposition). A mixture of 9.7 g I (R = OH), 8.65 g PhNHCOCH2-COMe, 40 ml AcOH, and 250 ml EtOH was boiled 5 hr and kept 2 days at 20° to yield 71.5% I [R = CH(COMe)CONHPh] (X), m. 202-3°. Reduction of X gave 53% I [R = CH(CH2NHPh)CHOHMe] (XI), hydrochloride m. 184° (decomposition). Heating a mixture of 5.7 g Ia and 50 ml concentrated H2SO4 2 hr at 100° yielded 89% Ia [:C(CN)CO2Et = :CHCONH2] (XII), m. 194.5-5.0°. Hydrogenation of XII gave 64% I (R = CH2CONH2) (XIII), m. 184.5-6.0° (EtOH). Reduction of XIII yielded 72.5% I (R = CH2CH2NH2) (XIV), hydrochloride m. 233° (decomposition). Boiling a mixture of 11.2 g I (R = OH), 4.75 g NCCH2CONH2, 40 ml AcOH and 250 ml EtOH 10 hr yielded 78% I [R = CH(CN)CONH2] (XV), m. 227° (decomposition). Reduction of XV gave 62.5% I [R = CH(CH2NH2)2], di-HCl, m. 254° (decomposition).

IT **26004-29-5P 26004-30-8P 26004-32-0P 26004-39-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

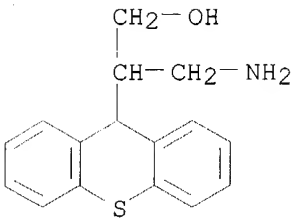
RN 26004-29-5 HCAPLUS
CN Xanthene-9-ethanol, β-(aminomethyl)- (8CI) (CA INDEX NAME)



RN 26004-30-8 HCAPLUS
CN Thioxanthene-9-ethanol, β-(aminomethyl)- (8CI) (CA INDEX NAME)

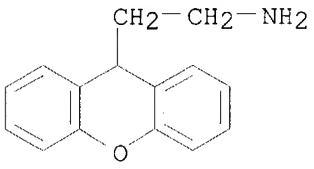


RN 26004-32-0 HCAPLUS
CN Thioxanthene-9-ethanol, β-(aminomethyl)-, hydrochloride (8CI) (CA INDEX NAME)



● HCl

RN 26004-39-7 HCAPLUS
CN Xanthene-9-ethylamine, hydrochloride (8CI) (CA INDEX NAME)



● HCl

L11 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:37664 HCAPLUS
DOCUMENT NUMBER: 70:37664
TITLE: Dibenzocycloalkanes, dibenzoxepins, and dibenzothiepins
PATENT ASSIGNEE(S): Boehringer, C. F., und Soehne G.m.b.H.
SOURCE: Brit., 16 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

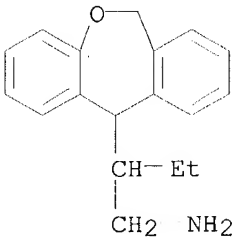
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1129029		19681002		
DE 1568089			DE	
FR 1513909			FR	

PRIORITY APPLN. INFO.: DE 19660311
GI For diagram(s), see printed CA Issue.
AB Tricyclic ketones condensed with nitriles gave hydroxy nitriles (I, R = H or alkyl, R1 = CN, R2 = OH), which were reduced to hydroxyethylamines (I, R = as above, R1 = CH2NH2, R2 = OH), dehydrated to II (R = H or alkyl, R1 = CH2NH2), and the exocyclic double bond hydrogenated; or the hydroxy nitriles were dehydrated and hydrogenated before reduction of CN to CH2NH2. MeCN (3.08 g.) and 10.5 g. 6,11-dihydrodibenzo-[b,e]oxepin-11-one were added to a solution of 2.3 g. Na and a trace of Fe(NO3)3 in 100 ml. liquid NH3, the mixture stirred 2 hrs., 6.4 g. NH4Cl added, followed by 80 ml. Et2O, NH3 evaporated, inorg. precipitate filtered off, Et2O evaporated, and the residue crystallized from C6H6 to give 32.8% 11-hydroxy-11-cyanomethyl-6,11-

134-5° (EtOAc), 92; O, H (XVI), 140-1° (iso-PrOH), 94.2; S, H, 72-3° (ligroine), 91; (CH2)2, H, 91-2° (iso-PrOH), 88; CH:CH, H, 102-3° (ligroine), 89; SCH2, H, 124-6° (EtOH), 94.5; -, Et, 81-2° (iso-PrOH), 69.5; O, Et, 113-14° (petroleum ether), 72; S, Et, 101-2° (iso-PrOH), 84.5; OCH2, Et, b0.2 165-70°, 81.2. Catalytic hydrogenation of 45 g. XVI in 500 ml. AcOH and 5 ml. H2SO4 in the presence of 2 g. Pt oxide for 4 hrs. gave 60% 9-(2-aminoethyl)xanthene (I, X = O, R = R2 = H, R1 = CH2NH2), b0.5 145-8°. XV was hydrogenated over Raney Ni catalyst to give I (X = bond line, R = R2 = H, R1 = CH2NH2), b0.2 131-5°, HCl salt m. 233-4°, in a 82-5% yield. Other I (R1 = CH2NH2, R2 = H) prepared by LiAl4 reduction of the corresponding cyanomethyl derivs. (X, R, b.p./mm., m.p. of salt, and % yield given): O, H, -, maleate 166-7°, 57.5; S, H, 160-2°/0.3, maleate 180°, 78; (CH2)2, H (XVII), 148-9°/0.1, HCl 237-8°, 84; CH:CH, H, -, HCl 238-40°, 80; OCH2, H, 163-4°/0.3, maleate 156°, 81; SCH2, H, -, HCl 251-2°, 67; -, Et, -, HCl 242-3°, 73; O, Et, -, HCl 251-2°, 98; S, Et, -, HCl 243-4°, 89; OCH2, Et, -, HCl 219-20°, 87. Hydrogenation of 23.5 g. IX in EtOH over Raney Ni in the presence of a trace of NaOH at 5 atmospheric gave 79% XVII. The ethylamines are pharmaceuticals with psychotropic and circulatory-stimulating activity.

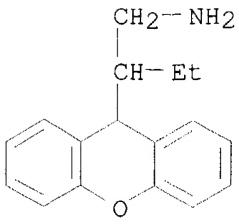
IT **21745-76-6P 21745-78-8P 21745-81-3P**
21745-82-4P 21745-83-5P 21745-84-6P
21745-85-7P 21745-86-8P 21745-88-0P
21761-61-5P 21828-95-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21745-76-6 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethylamine, β-ethyl-6,11-dihydro-, hydrochloride (8CI) (CA INDEX NAME)



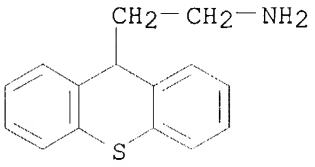
● HCl

RN 21745-78-8 HCAPLUS
CN Xanthene-9-ethylamine, β-ethyl-, hydrochloride (8CI) (CA INDEX NAME)

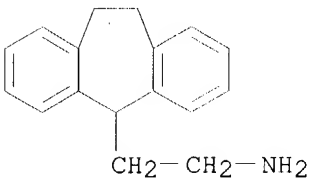


● HCl

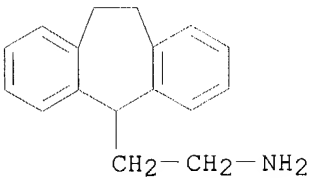
RN 21745-81-3 HCAPLUS
CN 9H-Thioxanthene-9-ethanamine (9CI) (CA INDEX NAME)



RN 21745-82-4 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro- (9CI) (CA INDEX NAME)

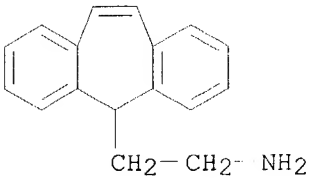


RN 21745-83-5 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)



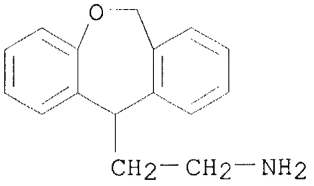
● HCl

RN 21745-84-6 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, hydrochloride (9CI) (CA INDEX NAME)

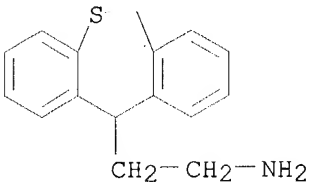


● HCl

RN 21745-85-7 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro- (9CI) (CA INDEX NAME)

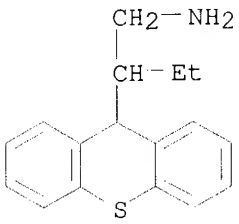


RN 21745-86-8 HCAPLUS
CN Dibenzo[b,e]thiepin-11-ethylamine, 6,11-dihydro-, hydrochloride (8CI) (CA INDEX NAME)



● HCl

RN 21745-88-0 HCAPLUS
CN Thioxanthene-9-ethylamine, β-ethyl-, hydrochloride (8CI) (CA INDEX NAME)



● HCl

RN 21761-61-5 HCAPLUS
CN Thioxanthene-9-ethylamine, maleate (8CI) (CA INDEX NAME)

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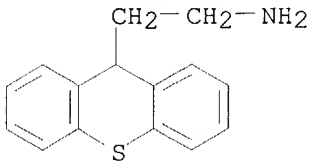
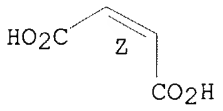
CRN 21745-81-3
CMF C15 H15 N S



CM 2

CRN 110-16-7
CMF C4 H4 O4

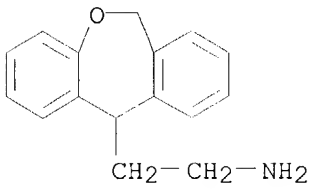
Double bond geometry as shown.



RN 21828-95-5 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethylamine, 6,11-dihydro-, maleate (8CI) (CA INDEX NAME)

CM 1

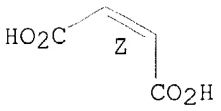
CRN 21745-85-7
CMF C16 H17 N O



CM 2

CRN 110-16-7
CMF C4 H4 O4

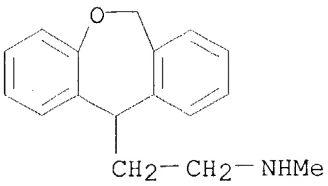
Double bond geometry as shown.



L11 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:28839 HCAPLUS
DOCUMENT NUMBER: 70:28839
TITLE: 11-(2-Dimethylaminoethyl)-6,11-dihydrodibenz[b,e]oxepins and -thiepins
PATENT ASSIGNEE(S): Boehringer, C. F., und Soehne G.m.b.H.
SOURCE: Brit., 3 pp. Division of Brit. 1129209
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1129210		19681002		
DE 1568104			DE	
FR 1518226			FR	

PRIORITY APPLN. INFO.: DE 19660409
GI For diagram(s), see printed CA Issue.
AB Division of Brit. 1,129,209. I are converted to II. Thus, a mixture of 6 g. 11-hydroxy-11-(N ,N -dimethyl-carbamoylmethyl) -6,11 - dihydrodibenz[b ,e]oxepin, 1.55 g. LiAlH4, and 50 ml. ether is agitated 4 hrs. at ≤10° and worked up to give 11-hydroxy-11(2-dimethylaminoethyl)-6, 11 - dihydrodibenz[b,e]oxepin, maleate m. 156-7°, HBr salt m. 214-15°. Similarly prepared are (starting material given): I(X = S, n = 1, R = OH), II(X = S, R = OH, R1 = Me) (III) (HCl salt m. 245°); I(X = O, n = 1, R = H), II(X = O, R = H, R1 = Me) (maleate m. 152-3°); I(X = S, n = 1, R = H), II(X = S, R = H, R1 = Me) (IV) (HCl salt m. 201-2°); V(X = CH2, n = 2, R = CONMe2), V(X = CH2, n = 2, R = CH2NMe2) (HCl salt m. 188-9°). III is heated with HCl(EtOH) to give V(X = S, n = 1, R = CH2NMe2), b0.05 160-2°; HCl salt m. 232-3°. IV is heated with ClCO2Et and the product is treated KOH to give II(X = O, R = H, R1 = H), HCl salt m. 215-16°. I(X = S, n = 2, R = OH) is treated with LiAlH4 and the product is dehydrated [HCl(EtOH)] to give V(X = S, n = 2, CH2NMe2), HCl salt m. 198-200°.
IT **21121-72-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21121-72-2 HCAPLUS
CN Dibenz[b,e]oxepin-11-ethylamine, 6,11-dihydro-N-methyl-, hydrochloride (8CI) (CA INDEX NAME)



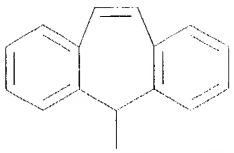
● HCl

L11 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1966:465380 HCAPLUS
DOCUMENT NUMBER: 65:65380
ORIGINAL REFERENCE NO.: 65:12150a-d
TITLE: Dibenzo[a,d]cycloheptene derivatives
INVENTOR(S): Judd, Claude I.; Drukker, Alexander E.; Biel, John H.
PATENT ASSIGNEE(S): Colgate-Palmolive Co.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3258488		19660628	US	19630812

AB Dibenzosuberene(I) (9.6 g.) in 75 cc. tetrahydrofuran treated in the cold with addition of 32 cc. 15.4% BuLi solution in 50 cc. Et2O, the solution stirred 4 hrs. at room temperature, and then 9 hrs. at room temperature with 6.1 g. 3-dimethylaminopropyl chloride in 30 cc. Et2O gave 10.85 g. 5-(3-dimethylaminopropyl)-5H-dibenzo[a,d]cycloheptene, b0.025 130-80°; maleate salt, m. 143-4° (alc.). Similarly, I with N-(3-chloropropyl)-N'-methylpiperazine gave 50% 5-(3-(4-methylpiperazino)propyl)-5H-dibenzo[a,d]cycloheptene, b0.06 182°; 2HCl salt, m. 262-4° (decomposition) (alc.-Et2O). Similarly, I and 1-(N-methyl-N-benzylamino)-3-chloropropane gave 70% 5-(3-N-methyl-N-benzylaminopropyl)-5H-dibenzo[a,d]-cycloheptene (II), b0.1 193-8°. II (32.7 g.), 11.2 g. Et chloroformate, and 80 ml. C6H6 refluxed 20 hrs. gave 5-(3-N-methyl-N-carbethoxyaminopropyl) -5H-dibenzo[a,d]cycloheptene (III). III (30 g.), 43.5 g. Ba(OH)2.8H2O, and 340 ml. (CH2OH)2 refluxed 10 hrs. gave 15.1 g. 5-(3-methylaminopropyl)-5Hdibenzo[a,d]cycloheptene, b0.35 163-4°; HCl, m. 170-1°. II (1.689 g.) in 150 ml. alc. hydrogenated at room temperature over 10% Pd-C gave 5-(3-methylaminopropyl)-5H-dibenzo[a,d]cycloheptene. The products are central stimulants and antispasmodics in animals.

IT **7186-44-9**, 5H-Dibenzo[a,d]cycloheptene-5-ethylamine, N-methyl-
(preparation of)
RN 7186-44-9 HCAPLUS
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, N-methyl- (9CI) (CA INDEX NAME)


CH2—CH2 NHMe

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 23 Jun 2004  VOL 140 ISS 26
FILE LAST UPDATED: 22 Jun 2004  (20040622/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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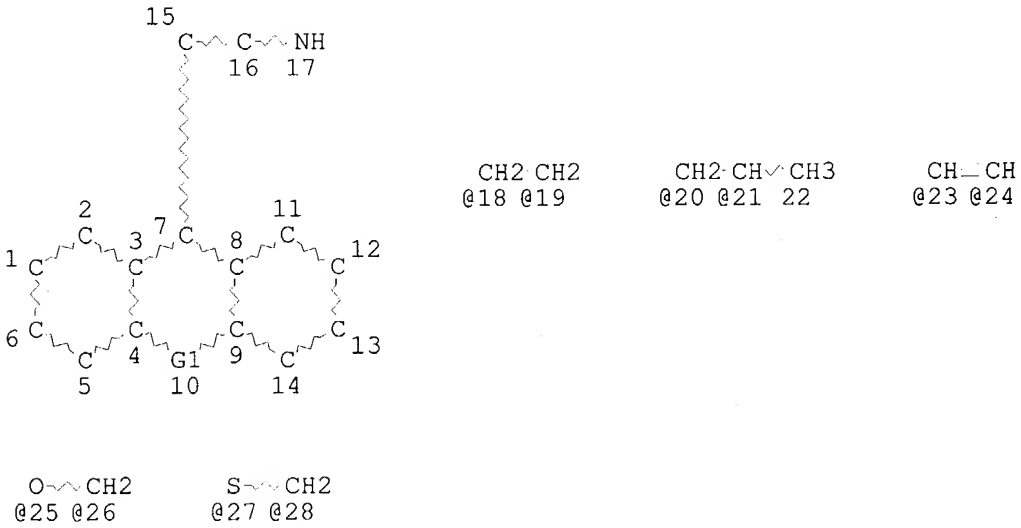


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8-9/28-4 27-9/O/S
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  28

STEREO ATTRIBUTES: NONE
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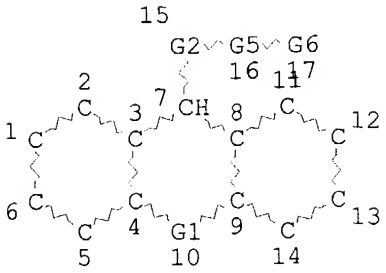

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CH~G7 @36 37 NH~CH3 @38 39 NH~Et @40 41

VAR G1=18-4 19-9/20-4 21-9/21-4 20-9/23-4 24-9/25-4 26-9/26-4 25-9/27-4 2
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE
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L11 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L10

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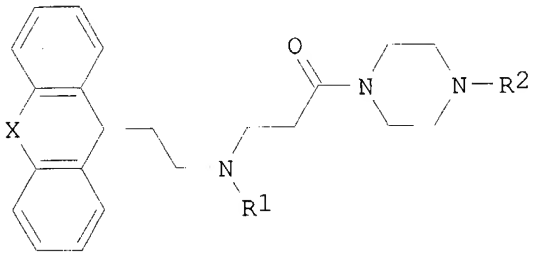
L11 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:376846 HCAPLUS
DOCUMENT NUMBER: 138:368918
TITLE: Preparation of piperazine derivatives having SST1 antagonistic activity
INVENTOR(S): Troxler, Thomas J.; Hoyer, Daniel
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma Gmbh
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2003040125 A1 20030515 WO 2002-EP12514 20021108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR
PRIORITY APPLN. INFO.: GB 2001-27008 A 20011109
OTHER SOURCE(S): MARPAT 138:368918
GI



I

AB The title compds. [I; X = a bond, O, S, CH2, CH:CH, CH2CH2; R1 = alkyl, alkenyl, (cycloalkyl)alkyl; R2 = (un)substituted Ph, 2-oxopyridyl, pyridyl, etc.] and their pharmaceutically acceptable acid addition salts, useful for the treatment of depression, anxiety and bipolar disorders, were prepared E.g., a multi-step synthesis of I [X = O; R1 = Me; R2 = 3,4-F2C6H3], starting from 9H-xanthen-9-ol and malonic acid, was given. The latter has high affinity for somatostatin receptors, independently of the species, and is SST1 selective. Its pKd values are as follows 8.3-8.8, 8.0-8.4, and 9.1 in human, mouse, and rat, resp.

IT **55286-76-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperazine derivs. having SST1 antagonistic activity)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:866076 HCAPLUS
DOCUMENT NUMBER: 138:106626
TITLE: Diastereoselective Synthesis of 2-Aminoalkyl-3-sulfonyl-1,3-oxazolidines on Solid Support
AUTHOR(S): Conde-Frieboes, Kilian; Schjeltved, Rie K.; Breinholt, Jens
CORPORATE SOURCE: Discovery Chemistry, Novo Nordisk A/S, Malov, DK-2760, Den.
SOURCE: Journal of Organic Chemistry (2002), 67(25), 8952-8957
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:106626

AB Herein we report our investigation on the oxidation of solid-support-bound amino alcs. to aldehydes. These aldehydes were converted to diastereomerically pure (>10:1) 2,4-cis-2-aminoalkyl-3-sulfonyl-1,3-oxazolidines using optically pure 1,2-amino alcs. The relative configuration was determined using the nuclear Overhauser effect. The synthesized oxazolidines, which were obtained in high purities, represent

a new, diverse scaffold for the solid-phase synthesis of libraries directed toward a pharmacol. target.

IT **488139-42-0P**
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(diastereoselective preparation of 2-(aminoalkyl)-3-sulfonyl-1,3-oxazolidines on solid support)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:830459 HCAPLUS
DOCUMENT NUMBER: 136:160841
TITLE: Structure-activity relationship studies on the potent multidrug resistance (MDR) modulator 2-(3,4-dimethoxyphenyl)-2-(methylethyl)-5-[(anthr-9-yl)methylamino]pentanenitrile (MM 36)
AUTHOR(S): Teodori, Elisabetta; Dei, Silvia; Garnier-Suillerot, Arlette; Quidu, Patricia; Scapecchi, Serena; Budriesi, Roberta
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita' di Firenze, Florence, 50121, Italy
SOURCE: Medicinal Chemistry Research (2001), 10(9), 563-576
CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser Boston
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A few derivs. of the potent MDR inhibitor 2-(3,4-dimethoxyphenyl)-2-(methylethyl)-5-[(anthr-9-yl)methylamino]pentanenitrile were synthesized and studied with the aim of optimizing activity and selectivity. Thus, even if dramatic improvements in potency and in selectivity were not reached, a better drug candidate and a new lead for further development of the series were identified.

IT **21745-81-3P**, 9H-Thioxanthene-9-ethanamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationship studies on potent multidrug resistance modulator 2-(3,4-dimethoxyphenyl)-2-(methylethyl)-5-[(anthr-9-yl)methylamino]pentanenitrile)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:66753 HCAPLUS
DOCUMENT NUMBER: 132:107773
TITLE: Preparation of aralkylamines as NMDA receptor-ionophore complex antagonists
INVENTOR(S): Mueller, Alan L.; Balandrin, Manuel F.; Vanwagenen, Bradford C.; Moe, Scott T.; Delmar, Eric G.; Artman, Linda D.; Barmore, Robert M.; Smith, Daryl L.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: U.S., 112 pp., Cont.-in-part of U.S. Ser. No. 663.013.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6017965	A	20000125	US 1996-763480	19961211
CA 2182680	AA	19950817	CA 1994-2182680	19941026
WO 9521612	A2	19950817	WO 1994-US12293	19941026

WO 9521612		A3	19950921	
W:	AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US			
RW:	KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
CN 1148337		A	19970423	CN 1994-195074 19941026
CN 1088585		B	20020807	
ES 2156162		T3	20010616	ES 1994-932057 19941026
EP 1123922		A2	20010816	EP 2000-121960 19941026
EP 1123922		A3	20040102	
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE			
PT 743853		T	20011031	PT 1994-932057 19941026
US 6071970		A	20000606	US 1995-485038 19950607
CA 2257234		AA	19971211	CA 1996-2257234 19961211
US 6211245		B1	20010403	US 1998-186341 19981104
AU 770292		B2	20040219	AU 2000-71810 20001124
US 2002004522		A1	20020110	US 2001-825373 20010402
US 6750244		B2	20040615	
JP 2004002437		A2	20040108	JP 2003-158350 20030603

PRIORITY APPLN. INFO.:

US 1993-14813	B2	19930208
US 1994-194210	B2	19940208
US 1994-288668	B2	19940809
WO 1994-US12293	A2	19941026
US 1995-485038	A2	19950607
US 1996-663013	A2	19960607
US 1994-288688	A2	19940811
EP 1994-932057	A3	19941026
JP 1995-521191	A3	19941026
WO 1996-US19525	A	19961206
AU 1997-13525	A3	19961211
US 1996-763480	A2	19961211
US 1997-869154	B2	19970604
US 1997-873011	A1	19970611
US 1998-186341	A1	19981104

OTHER SOURCE(S): MARPAT 132:107773

AB R7CHR4CR1R5CRR2R6[I; R = H or N(R3)2; R1,R5 = (un)substituted Ph, -CH2Ph, -OPh; R2,R6 = H or (hydroxy)alkyl; R1R2 = (CH2)n or (CH2)nNR3(CH2)n; R2R6 = NH; R3 = H, alkyl, CH2CH2OH, alkylphenyl; R4 = (un)substituted Ph, -pyridyl, -thienyl, etc.; R7 = (un)substituted Ph; n = 0-6] were prepared Thus, (3-FC6H4)2CO was condensed with (EtO)2P(O)CH2CO2Et and the product converted in 6 steps to (3-FC6H4)2CHCH2CHMeNH2. Data for biol. activity of I were given.

IT **14451-09-3P**, 5H-Dibenzo[a,d]cycloheptene-5-ethanamine **21745-77-7P**, 9H-Xanthene-9-ethanamine **21745-81-3P**, 9H-Thioxanthene-9-ethanamine **21745-82-4P 21745-83-5P 21745-85-7P 200430-08-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aralkylamines as NMDA receptor-ionophore complex antagonists)

REFERENCE COUNT: 172 THERE ARE 172 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:53380 HCAPLUS
DOCUMENT NUMBER: 132:93096
TITLE: Preparation of diarylalkylamines and related compounds active at both the serotonin reuptake site and the

N-methyl-D-aspartate receptor for treatment depression and other disorders.
INVENTOR(S): Mueller, Alan; Moe, Scott; Balandrin, Manuel
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 87 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000002551	A2	20000120	WO 1999-US15857	19990712
WO 2000002551	A3	20000921		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2336962	AA	20000120	CA 1999-2336962	19990712
AU 9949919	A1	20000201	AU 1999-49919	19990712
AU 771252	B2	20040318		
EP 1096926	A2	20010509	EP 1999-933987	19990712
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2004039014	A1	20040226	US 2001-990405	20011121

PRIORITY APPLN. INFO.: US 1998-92546P P 19980713
WO 1999-US15857 W 19990712

OTHER SOURCE(S): MARPAT 132:93096

AB A method for treatment of depression comprises administration of a compound having NMDA receptor binding activity of IC50 = 50 nM to 1 μM and serotonin reuptake IC50 ≤100 nM. The compds. include e.g. XmAr1(XmAr2)CHCR1R1CR2R2NR3R3 [X = Br, Cl, F, iodo, CF3, alkyl, OH, OCF3, alkoxy, acyloxy; Ar1, Ar2 = Ph, naphthyl, thiofuranyl, tetrahydronaphthyl, furyl, pyridyl, etc.; R1 = H, alkyl, hydroxyalkyl, OH, alkoxy, acyloxy; R2 = H, alkyl, hydroxyalkyl; (R2)2 = imino; R3 = H, alkyl, HOCH2CH2, alkylphenyl; m = 0-5]. Thus, N-methyl-bis-[3-(3-fluorophenyl)]propylamine (preparation given) at 5 mg/kg orally in mice produced a time-dependent reduction in the duration of immobility in the forced swimming test.

IT **21745-82-4P 21745-83-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diarylalkylamines and related compds. active at both the serotonin reuptake site and the N-methyl-D-aspartate receptor for treatment depression and other disorders)

L11 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:7958 HCAPLUS
DOCUMENT NUMBER: 130:66268
TITLE: Compounds active at a novel site on receptor-operated calcium channels useful for treatment of neurological disorders and diseases
INVENTOR(S): Mueller, Alan L.; Moe, Scott T.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 252 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9856752	A1	19981217	WO 1998-US11608	19980611
W: JP				
AU 770292	B2	20040219	AU 2000-71810	20001124

PRIORITY APPLN. INFO.: US 1997-873011 A 19970611
AU 1997-13525 A3 19961211

OTHER SOURCE(S): MARPAT 130:66268
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The compds. [I, II, III; R1 and R3 are independently selected from (un)substituted Ph, benzyl, phenoxy, H, alkyl, OH, etc.; R2 and R5 are independently selected from H, alkyl, hydroxyalkyl; R2-R5 together are imino; R1-R2 together are (CH2)n, (CH2)n-N(R6)-(CH2)n; n = 0-6, at least one n greater than 0; R6 is H, alkyl, 2-hydroxyethyl, and alkylphenyl; R4 is selected from (un)substituted thiofuryl, pyridyl, Ph, benzyl, phenoxy, phenylthio, H, alkyl, chcloalkyl; X, X1 is independently selected from (un)substituted Ph, benzyl, phenoxy, F, Cl, Br, Oh, etc.; m = 0-5; Y is N(R6)2, H when R1-R2 together are (CH2)n-N(R6)-(CH2)n], pharmaceutical compns., and pharmaceutical acceptable salts, complexes, and carriers are prepared as antagonists of NMDA receptor-mediated responses for treating a neurol. disease or disorder such as stroke, head trauma, spinal cord injury, spinal cord ischemia, ischemia- or hypoxia-induced nerve cell damage, epilepsy, anxiety, neuropsychiatric or cognitive deficits due to ischemia or hypoxia such as those that frequently occur as a consequence of cardiac surgery under cardiopulmonary bypass, or neurodegenerative diseases such as Alzheimer's Disease, Huntington's Disease, Parkinson's Disease, or amyotrophic lateral sclerosis (ALS).

IT **14451-09-3P**, 5H-Dibenzo[a,d]cycloheptene-5-ethanamine
21745-77-7P, 9H-Xanthene-9-ethanamine **21745-81-3P**,
9H-Thioxanthene-9-ethanamine **21745-82-4P 200429-81-8P**
200429-82-9P 200429-84-1P 200430-08-6P
217661-22-8P 217661-23-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(compds. active at novel site on receptor-operated calcium channels useful for treatment of neurol. disorders and diseases)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:1444 HCAPLUS
DOCUMENT NUMBER: 128:61341
TITLE: Preparation of aralkylamines as NMDA receptor-ionophore complex antagonists
INVENTOR(S): Mueller, Alan L.; Moe, Scott T.; Balandrin, Manuel F.; Vanwagenen, Bradford C.; Delmar, Eric G.; Artman, Linda D.; Barmore, Robert M.; Smith, Daryl L.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 298 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9746511	A1	19971211	WO 1996-US20697	19961211
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2257234	AA	19971211	CA 1996-2257234	19961211
AU 9713525	A1	19980105	AU 1997-13525	19961211
AU 723349	B2	20000824		
EP 912494	A1	19990506	EP 1996-945069	19961211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002511835	T2	20020416	JP 1998-500538	19961211
AU 770292	B2	20040219	AU 2000-71810	20001124

PRIORITY APPLN. INFO.: US 1996-663013 A 19960607
WO 1996-US19525 A 19961206
AU 1997-13525 A3 19961211
WO 1996-US20697 W 19961211

OTHER SOURCE(S): MARPAT 128:61341

AB R7CHR4CR1R5CRR2R6 [I; R = H or N(R3)2; R1,R5 = (un)substituted Ph, -CH2Ph, -OPh; R2,R6 = H or (hydroxy)alkyl; R1R2 = (CH2)n or (CH2)nNR3(CH2)n; R2R6 = NH; R3 = H, alkyl, CH2CH2OH, alkylphenyl; R4 = (un)substituted Ph, -pyridyl, -thienyl, etc.; R7 = (un)substituted Ph; n = 0-6] were prepared Thus, (3-FC6H4)2CO was condensed with (EtO)2P(O)CH2CO2Et and the product converted in 6 steps to (3-FC6H4)2CHCH2CHMeNH2. Data for biol. activity of I were given.

IT **14451-09-3P**, 5H-Dibenzo[a,d]cycloheptene-5-ethanamine **21745-77-7P**, 9H-Xanthene-9-ethanamine **21745-81-3P**, 9H-Thioxanthene-9-ethanamine **21745-82-4P 21745-83-5P 21745-85-7P 200429-81-8P 200429-82-9P 200429-83-0P 200429-84-1P 200429-85-2P 200430-08-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aralkylamines as NMDA receptor-ionophore complex antagonists)

L11 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:943447 HCAPLUS
DOCUMENT NUMBER: 123:339772
TITLE: Preparation of tricyclic tumor necrosis factor-α inhibitors
INVENTOR(S): Ting, Pauline C.; Friary, Richard J.; Tom, Wing C.; Lee, Joe F.; Seidl, Vera A.
PATENT ASSIGNEE(S): Schering Corp., USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

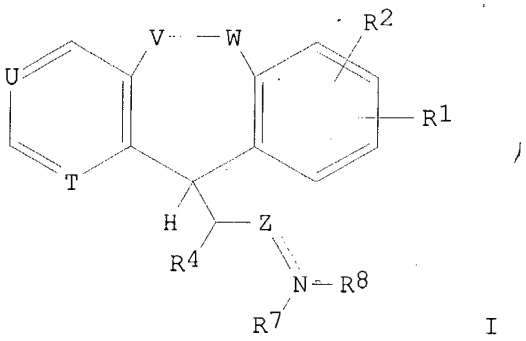
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9515959	A1	19950615	WO 1994-US13661	19941205
W: JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				

US 5574173	A	19961112	US 1993-162686	19931206
EP 733049	A1	19960925	EP 1995-903169	19941205
EP 733049	B1	19990310		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09500655	T2	19970121	JP 1994-516222	19941205
JP 2793914	B2	19980903		
AT 177425	E	19990315	AT 1995-903169	19941205
ES 2128701	T3	19990516	ES 1995-903169	19941205
CA 2175313	AA	19971030	CA 1996-2175313	19960429

PRIORITY APPLN. INFO.: US 1993-162686 19931206
WO 1994-US13661 19941205

OTHER SOURCE(S): MARPAT 123:339772

GI



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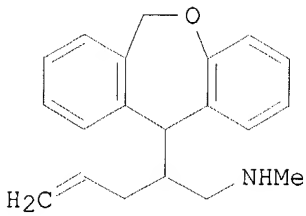


III

AB The title compds. [I; R1, R2 = H, halogen; R4 = alkenyl, alkoxy, OH; R7, R8 = H, alkyl, alkenyl, (un)substituted aryl, cycloalkyl, etc.; 1 of T and U is N and the other is :CH or both are :CH; 1 of V and W is O and the other is CH2 or both are CH2; Z = :CH, CH2, CH:CH, etc.; the dotted line is an optional double bond; NR7R8 = (un)substituted heterocyclyl], useful as tumor necrosis factor-α (II) inhibitors for treating septic shock, inflammation, or allergic diseases, are prepared and I-containing formulations presented. Thus, dibenzooxepine III was prepared and demonstrated 54% II inhibition at 10 μM.

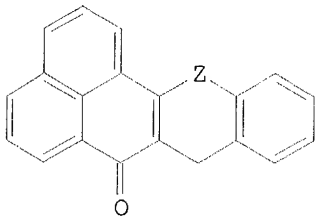
IT **170727-75-0P 170727-90-9P 170727-99-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tricyclic tumor necrosis factor-α inhibitors)

IT **170727-82-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tricyclic tumor necrosis factor-α inhibitors)

L11 ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:6529 HCAPLUS
DOCUMENT NUMBER: 96:6529
TITLE: Phenalenones. IV (1). Heterocycles from 3-hydroxyphenalenone (I)
AUTHOR(S): Kuroki, Masatane; Terachi, Yasuhito; Tsunashima,

	Yutaka
CORPORATE SOURCE:	Dep. Chem., Shibaura Inst. Technol., Ohmiya, 330, Japan
SOURCE:	Journal of Heterocyclic Chemistry (1981), 18(5), 873-6 CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 96:6529

GI



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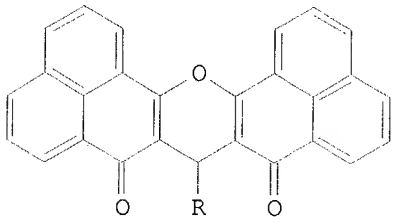


II

AB 3-Hydroxyphenalenone reacts with o-disubstituted benzenes (substituents: NH2, OH, CH2OH and SH), aliphatic and aromatic aldehydes to give various heterocyclic compds., e.g., I (Z = O, NH) and II (R = H, Me, aryl). These reactions resemble those of 1,3-cyclohexanediones in many respects.

IT **80090-01-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L11 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN

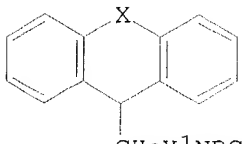
ACCESSION NUMBER:	1977:16562 HCAPLUS
DOCUMENT NUMBER:	86:16562
TITLE:	Amino alcohols with a tricyclic substituent
PATENT ASSIGNEE(S):	Boehringer Mannheim G.m.b.H., Fed. Rep. Ger.
SOURCE:	Fr. Demande, 13 pp. CODEN: FRXXBL
DOCUMENT TYPE:	Patent
LANGUAGE:	French
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

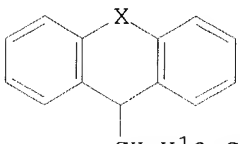
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2277589	A1	19760206	FR 1974-24202	19740711
FR 2277589	B1	19781229		

PRIORITY APPLN. INFO.: FR 1974-24202 19740711

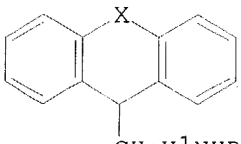
GI



I



II



III

IV

AB Aminopropanediols I (X = CH2O, X1 = CH2, CH2CH2, CHMe, R = Me, R1 = Ph; X = O, S, CH2CH2, CH:CH, X1 = CH2, R = Me, R1 = Ph; X = CH2CH2, X1 = CMe2, R = Et, R1 = Ph; X = X1 = CH2CH2, R = Me, R1 = Ph; X = CH2O, X1 = CH2, R = Et, R1 = Ph; X = CH2O, X1 = CH2, R = Me, R1 = cyclohexyl) were prepared by treating mesylates II with MeNHCH2CH(OH)CH2OPh or by treating the amines III with the glycidyl ethers IV. I at 0.5 mg/kg orally in dogs increased heart output by 20-67% over controls.

IT **21745-85-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of)

IT **7186-44-9P 55286-76-5P 55286-77-6P 55286-79-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phenyl glycidyl ether)

IT **55286-60-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phenylglycidyl ether)

IT **61257-18-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L11 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:546868 HCAPLUS
DOCUMENT NUMBER: 83:146868
TITLE: Carbonium ion reactions. XII. Acetolysis of 5-(2-bromoethyl)-5H-dibenzo[a,d]cycloheptene and nitrous acid deamination of 5-(2-aminoethyl)-5H-dibenzo[a,d]cycloheptene
AUTHOR(S): Banciu, M.; Badea, F.; Jelescu, Rodica; Cioranescu, Ecaterina
CORPORATE SOURCE: Lab. Org. Chem., Polytech. Inst., Bucharest, Rom.
SOURCE: Revue Roumaine de Chimie (1975), 20(1), 121-7
CODEN: RRCHAX; ISSN: 0035-3930
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The products formed in the acetolysis of I (R = Br) (II) and in the deamination of I (R = NH2) (III) were similar to those obtained in the acetolysis of I (R = p-MeC6H4SO3) (IV). The rearranged cycloheptene double bond in I increased from 37 to 87 to 100% in the series III < IV < II; the importance of this route increased with the decreasing efficiency of the leaving group. The kinetics of the acetolysis were discussed.

IT **14451-09-3**
RL: RCT (Reactant); RACT (Reactant or reagent)

(deamination of, mechanism of)
IT **21745-84-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L11 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:156136 HCAPLUS
DOCUMENT NUMBER: 82:156136
TITLE: 3-(Aryloxy)-2-hydroxypropylamine derivatives of tricyclic compounds as pharmaceuticals
INVENTOR(S): Winter, Werner; Thiel, Max; Stach, Kurt; Roesch, Egon; Sponer, Gisbert
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H.
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2335943	A1	19750130	DE 1973-2335943	19730714
DE 2335943	C3	19790809		
DE 2335943	B2	19781207		
US 3944566	A	19760316	US 1974-484353	19740628
CA 1026325	A1	19780214	CA 1974-204154	19740705
ZA 7404363	A	19750827	ZA 1974-4363	19740708
FI 7402110	A	19750115	FI 1974-2110	19740709
FI 59588	B	19810529		
FI 59588	C	19810910		
GB 1410755	A	19751022	GB 1974-30356	19740709
AU 7471032	A1	19760115	AU 1974-71032	19740709
AT 7405671	A	19760415	AT 1974-5671	19740709
AT 333756	B	19761210		
CH 602579	A	19780731	CH 1974-9531	19740710
SE 7409183	A	19750115	SE 1974-9183	19740712
SE 410594	B	19791022		
NL 7409439	A	19750116	NL 1974-9439	19740712
NL 184004	B	19881017		
NL 184004	C	19890316		
JP 50037766	A2	19750408	JP 1974-81039	19740715
JP 59005577	B4	19840206		

PRIORITY APPLN. INFO.: DE 1973-2335943 19730714
GI For diagram(s), see printed CA Issue.
AB Hydroxypropylamines I (X = CH2O, O, S, CH2CH2, CH:CH, X1 = CH2CH2, R = Me, R1 = Ph; X = CH2O, CH2CH2, X1 = (CH2)3, R = Me, R1 = Ph; X = CH2O, X1 = CH2CH2, R = Et, R1 = Ph, R = Me, R1 = cyclohexyl; X = CH2O, X1 = CHMeCH2, R = Me, R1 = Ph; X = CH2CH2, X1 = CH2CMe2, R = Et, R1 = Ph), active on the heart and circulation, were prepared .Thus, I (X = CH2O, X1 = CH2CH2, R = Me, R1 = Ph) was prepared by formylating 11-(2-aminoethyl)-6,11-dihydrodibenz[b,e]oxepin, reducing the formyl group, and treating the methylamine with phenyl glycidyl ether.
IT **21745-85-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of)
IT **55286-60-7P 55286-76-5P 55286-77-6P 55286-79-8P 55286-80-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phenyl glycidyl ether)
IT **55286-60-7**
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with cyclohexyl glycidyl ether)

L11 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:505324 HCAPLUS
DOCUMENT NUMBER: 81:105324
TITLE: Tricyclic aminoalcohols and their nontoxic salts
INVENTOR(S): Winter, Werner; Thiel, Max; Stach, Kurt; Schaumann, Wolfgang; Dietmann, Karl
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H.
SOURCE: Ger., 6 pp. Division of Ger. 1,568,145 (See Brit. 1,128,938 CA 70;47324u).
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1793735	A1	19730726	DE 1967-1793735	19670218
DE 1793735	B2	19740606		
DE 1793735	C3	19750130		
GB 1128938	A	19681002	GB 1967-33103	19670719

PRIORITY APPLN. INFO.: DE 1967-1793735 A 19670218
GI For diagram(s), see printed CA Issue.
AB Dibenzoxepinylethylamines I (X = O, R = cyclopentyl, cycloheptyl, cyclooctyl, cyclododecyl, 3-methylcyclohexyl, cyclohexylmethyl, 4-EtOC6H4, 3-MeC6H4, 3-O2N-C6H4CH2; X = S, R = 4-MeC6H4, 2-MeC6H4) were prepared in 54-81% yield by treating dibenzoxepinylethylamine with the epoxides II. II were prepared by treating epichlorohydrin with RXH. I enhance cardiac blood flow and are β-sympatholytics. Thus I (X = O, R = 4-EtOC6H4) at 0.5 mg/kg orally increased cardiac blood flow in dogs by 275%.
IT **21745-85-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with epoxy propanes)
IT **53444-66-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with epoxypropane derivs.)

L11 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1970:100435 HCAPLUS
DOCUMENT NUMBER: 72:100435
TITLE: Synthesis of aminoalkylxanthenes and aminothioxanthenes
AUTHOR(S): Tsvetkova, I. D.; Orlova, E. K.; Zagorevskii, V. A.
CORPORATE SOURCE: Inst. Farmakol. Khimioter., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1969), 3(12), 17-20
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Derivs. of xanthene (I) and thioxanthene (II) were prepared Hydrogenation of Ia over Pd yielded 79.5% I [R = CH(CN)CO2Et] (III), m. 127-8°. Reduction of III with LiAlH4 gave 75% I [R = CH(CH2OH)CH2NH2] (IV), m. 115.5-16°; HCl salt m. 234-5°. Analogously, II [R = CH(CN)CO2Et] yielded 90% II [R = CH(CH2OH)CH2NH2] (V), m. 112.5-13°; HCl salt m. 215° (decomposition). A mixture of 0.5 g IV, 0.92 g HCO2H and 2 ml H2CO was boiled 7 hr and saturated with HCl to yield 55% I [R = CH(CH2OH)CH2NMe2·HCl] (VI), 192° (decomposition). Treatment of VI with MeCOCl gave 96% I [R = CH(CH2O2CMe)CH2NMe2·HCl] (VII), m. 179-80° (decomposition). Boiling II [R = CH(CN)CO2Et] with C5H11N yielded 75% II [R = CH(CN)CONC5H10] (VIII), m. 190-1°

(EtOH). Reduction of VIII with LiAlH4 gave 18% II [R = CH(CH2NC5H10)CH2NH2·2HCl] (IX), m. 250° (decomposition). A mixture of 9.7 g I (R = OH), 8.65 g PhNHCOCH2-COMe, 40 ml AcOH, and 250 ml EtOH was boiled 5 hr and kept 2 days at 20° to yield 71.5% I [R = CH(COMe)CONHPh] (X), m. 202-3°. Reduction of X gave 53% I [R = CH(CH2NHPh)CHOHMe] (XI), hydrochloride m. 184° (decomposition). Heating a mixture of 5.7 g Ia and 50 ml concentrated H2SO4 2 hr at 100° yielded 89% Ia [:C(CN)CO2Et = :CHCONH2] (XII), m. 194.5-5.0°. Hydrogenation of XII gave 64% I (R = CH2CONH2) (XIII), m. 184.5-6.0° (EtOH). Reduction of XIII yielded 72.5% I (R = CH2CH2NH2) (XIV), hydrochloride m. 233° (decomposition). Boiling a mixture of 11.2 g I (R = OH), 4.75 g NCCH2CONH2, 40 ml AcOH and 250 ml EtOH 10 hr yielded 78% I [R = CH(CN)CONH2] (XV), m. 227° (decomposition). Reduction of XV gave 62.5% I [R = CH(CH2NH2)2], di-HCl, m. 254° (decomposition).

IT **26004-29-5P 26004-30-8P 26004-32-0P 26004-39-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L11 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:37664 HCAPLUS
DOCUMENT NUMBER: 70:37664
TITLE: Dibenzocycloalkanes, dibenzoxepins, and dibenzothiepins
PATENT ASSIGNEE(S): Boehringer, C. F., und Soehne G.m.b.H.
SOURCE: Brit., 16 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1129029		19681002		
DE 1568089			DE	
FR 1513909			FR	

PRIORITY APPLN. INFO.: DE 19660311
GI For diagram(s), see printed CA Issue.
AB Tricyclic ketones condensed with nitriles gave hydroxy nitriles (I, R = H or alkyl, R1 = CN, R2 = OH), which were reduced to hydroxyethylamines (I, R = as above, R1 = CH2NH2, R2 = OH), dehydrated to II (R = H or alkyl, R1 = CH2NH2), and the exocyclic double bond hydrogenated; or the hydroxy nitriles were dehydrated and hydrogenated before reduction of CN to CH2NH2. MeCN (3.08 g.) and 10.5 g. 6,11-dihydrodibenzo-[b,e]oxepin-11-one were added to a solution of 2.3 g. Na and a trace of Fe(NO3)3 in 100 ml. liquid NH3, the mixture stirred 2 hrs., 6.4 g. NH4Cl added, followed by 80 ml. Et2O, NH3 evaporated, inorg. precipitate filtered off, Et2O evaporated, and the residue crystallized from C6H6 to give 32.8% 11-hydroxy-11-cyanomethyl-6,11-dihydrodibenzo[b,e]oxepin (I, X = OCH2, R = H, R1 = CN, R2 = OH) (III), m. 147-8°. The use of Li instead of Na gave pure III in 90.5% yield. Other I (R1 = CN, R2 = OH) prepared similarly are (X, R, m.p., and % yield given): bond line, H, 110-11° (petroleum ether), 65; O, H, 137-8° (petroleum ether), 73; S, H (IV), 127-8° (ligroine), 77; CH:CH, H (V), 202-4° (EtOH), 73; SCH2, H, 119-20° (C6H6-hexane), 53; (CH2)3, H, 161-3° (iso-PrOH), 46; S(CH2)2, H, 143-5° (EtOH), 57.7 (impure); CO, H, 170-1° (iso-PrOH), 64.5; -, Et, 133-5° (ligroine), 83; O, Et, 106-7° (ligroine), 100 (impure); S, Et, 103-4° (iso-PrOH), 95 (impure); CH:CH, Et, 161-2° (EtOH), 92 (impure); OCH2, Et, 158-9° (C6H6), 65; SCH2, Et, -, -; (CH2)3, Et, 115-16° (iso-PrOH), 36. IV (18.5 g.) was reduced with LiAlH4 to 9-hydroxy-9-(2-

aminoethyl)thiaxanthene (I, X = S, R = H, R1 = CH2NH2, R2 = OH), m. 188° (iso-PrOH), in 61% yield. Other I (R1 = CH2NH2, R2 = OH) prepared similarly are (X, R, m.p., % yield, m.p. of HCl salt, and % yield of HCl salt given): bond line, H, 114°, 52, -, -; CH:CH, H, 156-8°, 82, -, -; OCH2, H, -, -, 110-15°, 69; SCH2, H, 118-19°, -, 113-15°, 58; (CH2)3, H, -, -, 190-200°, 44; S(CH2)2, H, -, 50, 208°, -; CO, H, -, -, 184-5°, 68.5; -, Et, -, 83.5, 215°, -; O, Et, 134-5°, 79.5, -, -; S, Et, -, 81.5, 204-5°, -; CH:CH, Et (VI), 139-40°, 70.4, 294° (decomposition), -; OCH2, Et (VII), -, 69.5, 227-8°, -; SCH2, Et, -, 54, 253°, -; (CH2)3, Et, -, -, 249-50°, -. VI (11.3 g.) in 100 ml. 48% HBr was heated 1 hr. at 100° to give 68% 5-(1-amino-2-butylidene)dibenzo[a,d]cycloheptene (II, X = CH:CH, R = Et, R1 = CH2NH2) (VIII). b0.2 160-2°; HCl salt m. 194-5° (iso-PrOH). Similarly prepd, with HBr in AcOH was 91% II·HCl (X = bond line, R = Et, R1 = CH2NH2), m. 239°. VII·HCl (12 g.) in 50 ml. EtOH saturated with HCl was boiled 1 hr. to give 86.7% II·HCl (X = OCH2, R = Et, R1 = CH2NH2), m. 223-4° (iso-PrOH). Other II·HCl (R1 = CH2NH2) prepared similarly are (X, R, m.p. of HCl salt, and % yield given): bond line, H, 268-70°, 60.1; O, H, 175°, 93; S, H, 183-4°, 90.2; (CH2)2, H (IX), 208-9°, 59.5; CH:CH, H, 232-3°, 65.5; OCH2, H (X), 235-7°, 37.1; SCH2, H, 217-18°, 83; (CH2)3, H, 243-5°, 47.5; S, Et, 232-3°, 84; (CH2)2, Et (XI), 219-20°, 79.5; SCH2, Et, 267°, 93.5; (CH2)3, Et, 271-2°, 78.5. V (10 g.) in 150 ml. iso-PrOH saturated with HCl was boiled 1 hr. to give 79% 5-cyanomethylene-5H-dibenzo[a,d]cycloheptene (II, X = CH:CH, R = H, R1 = CN), m. 143-4° (ligroine). Other II (R1 = CN) prepared by heating the corresponding I (R1 = CN, R2 = OH) are (X, R, b.p./mm., m.p., % yield, and dehydrating agent given): (CH2)3, H (XII), 182-3°/0.8, 64-5° (petroleum ether), 63, HCl/EtOH; -, H, 155-64°/0.05, 110-11°, 78.1, P2O5; O, H, 196-200°/0.4, 134-5°, 87.4, HCl/EtOH; S, H, -, 156-8°, 91.1, HCl/EtOH; (CH2)2, H, -, 105-6°, 81, HCl/EtOH; OCH2, H (XIII), -, 150-1°, 67.6, HCl/EtOH; SCH2, H, -, 176-7°, 83.5, HCl/EtOH; CO, H, -, 191-2°, 60, (CO2)H2; bond line, Et, 170-1°/0.1, 77-8°, 92, P2O5; O, Et, 160-2°/10.2, 82-3°, (petroleum ether), 57.8, P2O5; O, Et, 170-5°/0.1, 79-80°, 80.5, HCl/EtOH; S, Et, -, 106-7°, 85.5, HCl/EtOH; (CH2)2, Et (XIV), 173-85°/ 0.1, 86-8°, 89.5, HCl/EtOH; CH:CH, Et, -, 141-2°, 74.5, P2O5; OCH2, Et, -, 126-7°, 73.5, HCl/EtOH; SCH2, Et, -, 112-13°, 62.5, HCl/EtOH. In the preparation of XII, 36% 5,6,7,12-tetrahydrodibenzo[a,d]cycloocten-12-one, b0.8 173-8°, was obtained as a by-product. LiAlH4 reduction of XIV gave 70.6% XI, m. 224-5° (EtOH-Et2O). Similarly prepared were 76.4% VIII; 73% IX, b0.15 151-2°; 56% X; and 49% II (X = O, R = Et, R1 = CH2NH2), HCl salt m. 187-8°. Reduction of 12 g. XIII with Al amalgam gave 95.5% 11-cyanomethyl-6, 11-dihydrodibenzo-[b,e]oxepin (I, X = OCH2, R = R2 = H, R1 = CN), m. 87-9° (ligroine). Other I (R1 = CN, R2 = H) prepared similarly are (X, R, m.p., and % yield given): bond line, H (XV), 134-5° (EtOAc), 92; O, H (XVI), 140-1° (iso-PrOH), 94.2; S, H, 72-3° (ligroine), 91; (CH2)2, H, 91-2° (iso-PrOH), 88; CH:CH, H, 102-3° (ligroine), 89; SCH2, H, 124-6° (EtOH), 94.5; -, Et, 81-2° (iso-PrOH), 69.5; O, Et, 113-14° (petroleum ether), 72; S, Et, 101-2° (iso-PrOH), 84.5; OCH2, Et, b0.2 165-70°, 81.2. Catalytic hydrogenation of 45 g. XVI in 500 ml. AcOH and 5 ml. H2SO4 in the presence of 2 g. Pt oxide for 4 hrs. gave 60% 9-(2-aminoethyl)xanthene (I, X = O, R = R2 = H, R1 = CH2NH2), b0.5 145-8°. XV was hydrogenated over Raney Ni catalyst to give I (X = bond line, R = R2 = H, R1 = CH2NH2), b0.2 131-5°, HCl salt m. 233-4°, in a 82-5% yield. Other I (R1 = CH2NH2, R2 = H) prepared by LiAl4 reduction of the corresponding cyanomethyl derivs. (X, R, b.p./mm., m.p. of salt, and % yield given): O, H, -, maleate 166-7°, 57.5; S,

H, 160-2°/0.3, maleate 180°, 78; (CH2)2, H (XVII), 148-9°/0.1, HCl 237-8°, 84; CH:CH, H, -, HCl 238-40°, 80; OCH2, H, 163-4°/0.3, maleate 156°, 81; SCH2, H, -, HCl 251-2°, 67; -, Et, -, HCl 242-3°, 73; O, Et, -, HCl 251-2°, 98; S, Et, -, HCl 243-4°, 89; OCH2, Et, -, HCl 219-20°, 87. Hydrogenation of 23.5 g. IX in EtOH over Raney Ni in the presence of a trace of NaOH at 5 atmospheric gave 79% XVII. The ethylamines are pharmaceuticals with psychotropic and circulatory-stimulating activity.

IT **21745-76-6P 21745-78-8P 21745-81-3P**
21745-82-4P 21745-83-5P 21745-84-6P
21745-85-7P 21745-86-8P 21745-88-0P
21761-61-5P 21828-95-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L11 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:28839 HCAPLUS
DOCUMENT NUMBER: 70:28839
TITLE: 11-(2-Dimethylaminoethyl)-6,11-dihydrodibenz[b,e]oxepins and -thiepins
PATENT ASSIGNEE(S): Boehringer, C. F., und Soehne G.m.b.H.
SOURCE: Brit., 3 pp. Division of Brit. 1129209
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1129210		19681002		
DE 1568104			DE	
FR 1518226			FR	

PRIORITY APPLN. INFO.: DE 19660409
GI For diagram(s), see printed CA Issue.
AB Division of Brit. 1,129,209. I are converted to II. Thus, a mixture of 6 g. 11-hydroxy-11-(N ,N -dimethyl-carbamoylmethyl) -6,11 - dihydrodibenz[b ,e]oxepin, 1.55 g. LiAlH4, and 50 ml. ether is agitated 4 hrs. at ≤10° and worked up to give 11-hydroxy-11(2-dimethylaminoethyl)-6, 11 - dihydrodibenz[b,e]oxepin, maleate m. 156-7°, HBr salt m. 214-15°. Similarly prepared are (starting material given): I(X = S, n = 1, R = OH), II(X = S, R = OH, R1 = Me) (III) (HCl salt m. 245°); I(X = O, n = 1, R = H), II(X = O, R = H, R1 = Me) (maleate m. 152-3°); I(X = S, n = 1, R = H), II(X = S, R = H, R1 = Me) (IV) (HCl salt m. 201-2°); V(X = CH2, n = 2, R = CONMe2), V(X = CH2, n = 2, R = CH2NMe2) (HCl salt m. 188-9°). III is heated with HCl(EtOH) to give V(X = S, n = 1, R = CH2NMe2), b0.05 160-2°; HCl salt m. 232-3°. IV is heated with ClCO2Et and the product is treated KOH to give II(X = O, R = H, R1 = H), HCl salt m. 215-16°. I(X = S, n = 2, R = OH) is treated with LiAlH4 and the product is dehydrated [HCl(EtOH)] to give V(X = S, n = 2, CH2NMe2), HCl salt m. 198-200°.

IT **21121-72-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L11 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1966:465380 HCAPLUS
DOCUMENT NUMBER: 65:65380
ORIGINAL REFERENCE NO.: 65:12150a-d
TITLE: Dibenzo[a,d]cycloheptene derivatives
INVENTOR(S): Judd, Claude I.; Drukker, Alexander E.; Biel, John H.

PATENT ASSIGNEE(S): Colgate-Palmolive Co.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3258488		19660628	US	19630812

AB Dibenzosuberene(I) (9.6 g.) in 75 cc. tetrahydrofuran treated in the cold with addition of 32 cc. 15.4% BuLi solution in 50 cc. Et2O, the solution stirred 4 hrs. at room temperature, and then 9 hrs. at room temperature with 6.1 g. 3-dimethylaminopropyl chloride in 30 cc. Et2O gave 10.85 g. 5-(3-dimethylaminopropyl)-5H-dibenzo[a,d]cycloheptene, b0.025 130-80°; maleate salt, m. 143-4° (alc.). Similarly, I with N-(3-chloropropyl)-N'-methylpiperazine gave 50% 5-(3-(4-methylpiperazino)propyl)-5H-dibenzo[a,d]cycloheptene, b0.06 182°; 2HCl salt, m. 262-4° (decomposition) (alc.-Et2O). Similarly, I and 1-(N-methyl-N-benzylamino)-3-chloropropane gave 70% 5-(3-N-methyl-N-benzylaminopropyl)-5H-dibenzo[a,d]-cycloheptene (II), b0.1 193-8°. II (32.7 g.), 11.2 g. Et chloroformate, and 80 ml. C6H6 refluxed 20 hrs. gave 5-(3-N-methyl-N-carbethoxyaminopropyl) -5H-dibenzo[a,d]cycloheptene (III). III (30 g.), 43.5 g. Ba(OH)2.8H2O, and 340 ml. (CH2OH)2 refluxed 10 hrs. gave 15.1 g. 5-(3-methylaminopropyl)-5Hdibenzo[a,d]cycloheptene, b0.35 163-4°; HCl, m. 170-1°. II (1.689 g.) in 150 ml. alc. hydrogenated at room temperature over 10% Pd-C gave 5-(3-methylaminopropyl)-5H-dibenzo[a,d]cycloheptene. The products are central stimulants and antispasmodics in animals.

IT **7186-44-9**, 5H-Dibenzo[a,d]cycloheptene-5-ethylamine, N-methyl-
(preparation of)

=>
=> => fil caold
FILE 'CAOLD' ENTERED AT 14:44:05 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=>
=>

=> s l10
L12 1 L10

=> d all l12 1

L12 ANSWER 1 OF 1 CAOLD COPYRIGHT 2004 ACS on STN

AN CA65:12150a CAOLD
TI 6-dimethyl-6-halomethyl-5a,6-anhydrotetracyclines
AU Blackwood, Robert K.; Rennhard, H. H.; Beereboom, J. J.; Stephens, C. R., Jr.
PA Pfizer, Chas., & Co., Inc.
DT Patent
TI dibenzo[a,d]cycloheptene derivs.
AU Judd, Claude I.; Drukker, A. E.; Biel, J. H.
DT Patent

	PATENT NO.	KIND	DATE
PI	US 3258488		1966
PI	US 3264348		1966

IT 81-50-5 128-93-8 2022-93-7 3241-90-5 3241-91-6 3241-92-7
3241-93-8 3241-95-0 3548-66-1 3596-13-2 3596-21-2 3596-32-5
3765-10-4 3896-76-2 4028-89-1 4574-51-0 4878-87-9 5115-20-8
6746-03-8 7186-17-6 7186-39-2 7186-40-5 **7186-44-9**
7196-42-1 13202-77-2 19283-16-0 35764-89-7

=>
=>

=> fil reg
FILE 'REGISTRY' ENTERED AT 14:44:18 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7
DICTIONARY FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

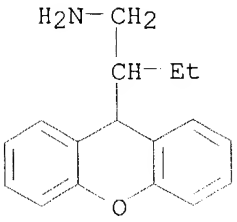
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

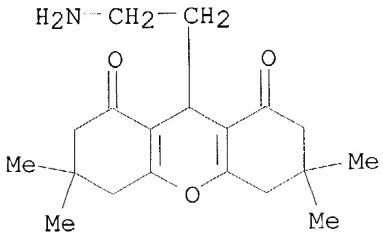
=> d ide can l10 tot

L10 ANSWER 1 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 686701-25-7 REGISTRY
CN 9H-Xanthene-9-ethanamine, β-ethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H19 N O
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 2 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 488139-42-0 REGISTRY
CN 1H-Xanthene-1,8(2H)-dione, 9-(2-aminoethyl)-3,4,5,6,7,9-hexahydro-3,3,6,6-tetramethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H27 N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: CMBI (Combinatorial study); PREP (Preparation)

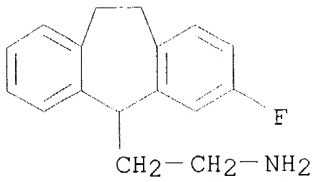


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:106626

L10 ANSWER 3 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 217661-23-9 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-fluoro-10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)
MF C17 H18 F N . Cl H
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
CRN (200429-85-2)

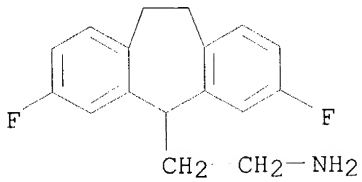


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:66268

L10 ANSWER 4 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 217661-22-8 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3,7-difluoro-10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)
MF C17 H17 F2 N . Cl H
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
CRN (200429-83-0)

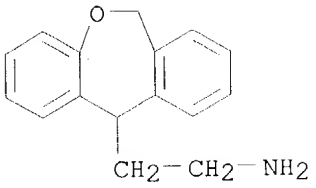


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:66268

L10 ANSWER 5 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 200430-08-6 REGISTRY
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)
MF C16 H17 N O . Cl H
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
CRN (21745-85-7)



● HCl

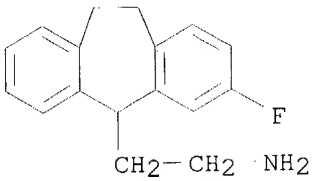
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:107773

REFERENCE 2: 130:66268

REFERENCE 3: 128:61341

L10 ANSWER 6 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 200429-85-2 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H18 F N
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



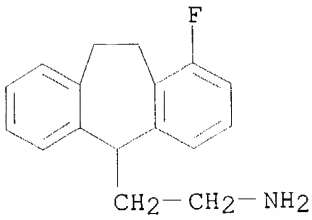
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:61341

L10 ANSWER 7 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 200429-84-1 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1-fluoro-10,11-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H18 F N
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES

(Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:66268

REFERENCE 2: 128:61341

L10 ANSWER 8 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 200429-83-0 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3,7-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H17 F2 N
CI COM
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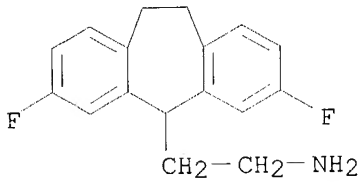
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



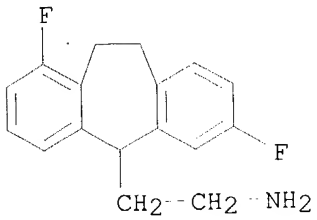
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:61341

L10 ANSWER 9 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 200429-82-9 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1,7-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H17 F2 N
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



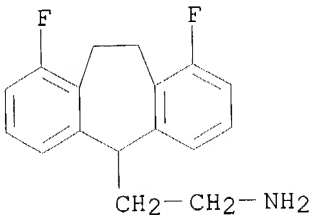
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:66268

REFERENCE 2: 128:61341

L10 ANSWER 10 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 200429-81-8 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 1,9-difluoro-10,11-dihydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H17 F2 N
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

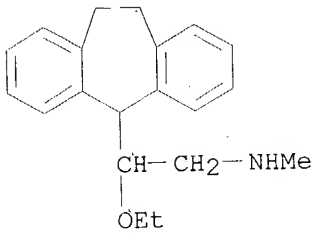
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:66268

REFERENCE 2: 128:61341

L10 ANSWER 11 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 170727-99-8 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, β-ethoxy-10,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H25 N O

SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

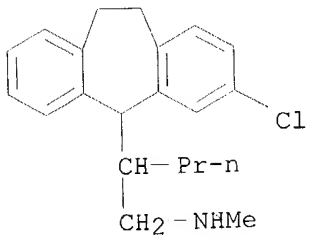
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 123:339772

L10 ANSWER 12 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 170727-90-9 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-chloro-10,11-dihydro-N-methyl-β-propyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-chloro-10,11-dihydro-N-methyl-β-propyl-, (Z)-2-butenedioate (1:1)
FS STEREOSEARCH
MF C21 H26 Cl N . C4 H4 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

CM 1

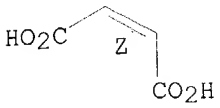
CRN 170727-89-6
CMF C21 H26 Cl N



CM 2

CRN 110-16-7
CMF C4 H4 O4

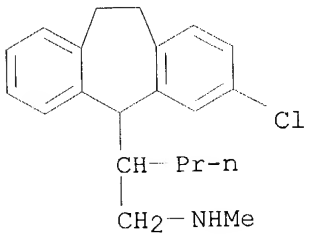
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 123:339772

L10 ANSWER 13 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 170727-89-6 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 3-chloro-10,11-dihydro-N-methyl-β-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H26 Cl N
CI COM
SR CA

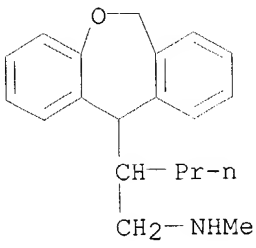


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 14 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 170727-82-9 REGISTRY
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl-β-propyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl-β-propyl-, (Z)-2-butenedioate (1:1)
FS STEREOSEARCH
MF C20 H25 N O . C4 H4 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: RACT (Reactant or reagent)

CM 1

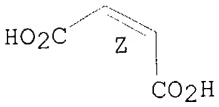
CRN 170727-75-0
CMF C20 H25 N O



CM 2

CRN 110-16-7
CMF C4 H4 O4

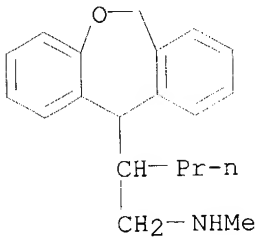
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 123:339772

L10 ANSWER 15 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 170727-75-0 REGISTRY
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl-β-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H25 N O
CI COM
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

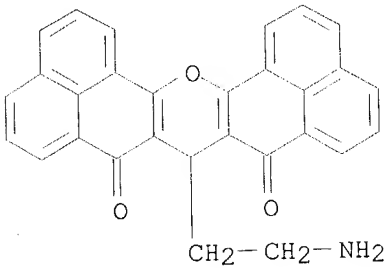


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 123:339772

L10 ANSWER 16 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 80090-01-3 REGISTRY
CN 7H,8H,9H-Dinaphtho[1,8-bc:1',8'-hi]xanthene-7,9-dione, 8-(2-aminoethyl)-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H19 N O3
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

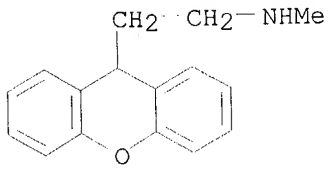


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 96:6529

L10 ANSWER 17 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 61257-18-9 REGISTRY
CN 9H-Xanthene-9-ethanamine, N-methyl-, hydrochloride (9CI) (CA INDEX NAME)
MF C16 H17 N O . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)
CRN (55286-76-5)



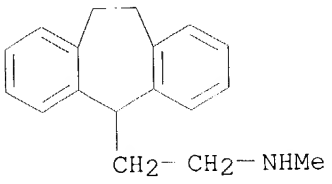
● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 86:16562

L10 ANSWER 18 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55286-80-1 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro-N-methyl- (9CI)

(CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 N
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

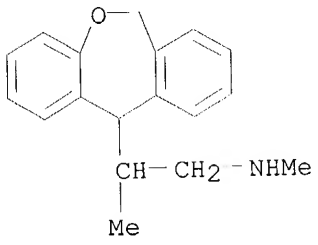


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 82:156136

L10 ANSWER 19 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55286-79-8 REGISTRY
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N,β-dimethyl- (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 N O
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

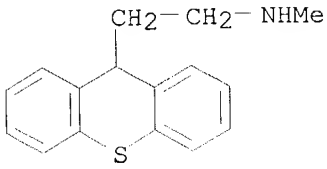
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 86:16562

REFERENCE 2: 82:156136

L10 ANSWER 20 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55286-77-6 REGISTRY
CN 9H-Thioxanthene-9-ethanamine, N-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N S
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



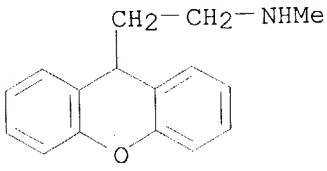
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 86:16562

REFERENCE 2: 82:156136

L10 ANSWER 21 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55286-76-5 REGISTRY
CN 9H-Xanthene-9-ethanamine, N-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N O
CI COM
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

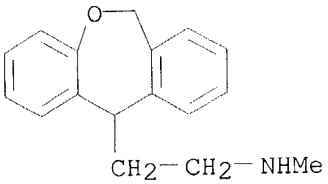
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:368918

REFERENCE 2: 86:16562

REFERENCE 3: 82:156136

L10 ANSWER 22 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55286-60-7 REGISTRY
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro-N-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H19 N O
CI COM
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



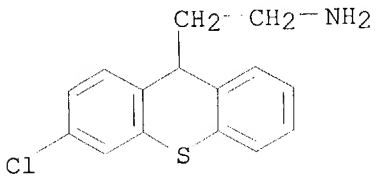
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 86:16562

REFERENCE 2: 82:156136

L10 ANSWER 23 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 53444-66-9 REGISTRY
CN 9H-Thioxanthene-9-ethanamine, 3-chloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H14 Cl N S
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: RACT (Reactant or reagent)

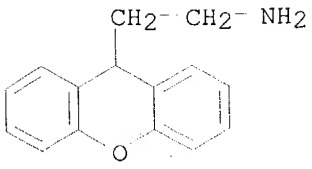


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 81:105324

L10 ANSWER 24 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 26004-39-7 REGISTRY
CN Xanthene-9-ethylamine, hydrochloride (8CI) (CA INDEX NAME)
MF C15 H15 N O . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
CRN (21745-77-7)

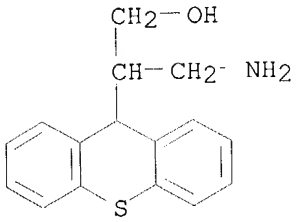


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 72:100435

L10 ANSWER 25 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 26004-32-0 REGISTRY
CN Thioxanthene-9-ethanol, β-(aminomethyl)-, hydrochloride (8CI) (CA INDEX NAME)
MF C16 H17 N O S . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
CRN (26004-30-8)

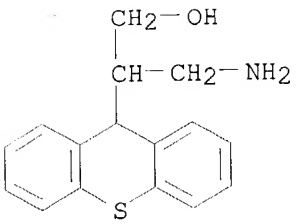


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 72:100435

L10 ANSWER 26 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 26004-30-8 REGISTRY
CN Thioxanthene-9-ethanol, β-(aminomethyl)- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N O S
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

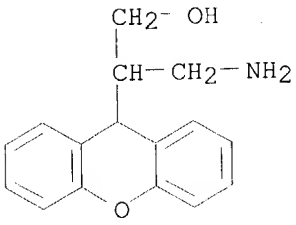


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 72:100435

L10 ANSWER 27 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 26004-29-5 REGISTRY
CN Xanthene-9-ethanol, β-(aminomethyl)- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

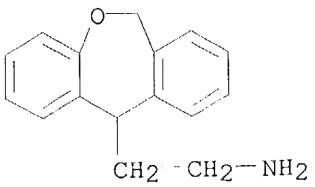
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 72:100435

L10 ANSWER 28 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21828-95-5 REGISTRY
CN Dibenz[b,e]oxepin-11-ethylamine, 6,11-dihydro-, maleate (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H17 N O . x C4 H4 O4
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)

CM 1

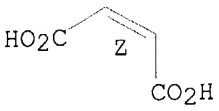
CRN 21745-85-7
CMF C16 H17 N O



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



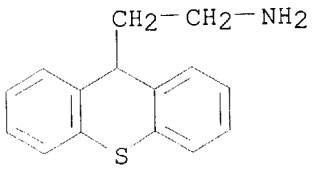
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:37664

L10 ANSWER 29 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21761-61-5 REGISTRY
CN Thioxanthene-9-ethylamine, maleate (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H15 N S . x C4 H4 O4
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)

CM 1

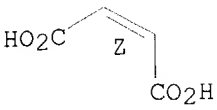
CRN 21745-81-3
CMF C15 H15 N S



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



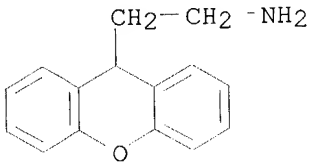
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:37664

L10 ANSWER 30 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21761-60-4 REGISTRY
CN Xanthene-9-ethylamine, maleate (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H15 N O . x C4 H4 O4

CM 1

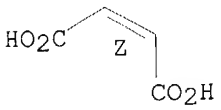
CRN 21745-77-7
CMF C15 H15 N O



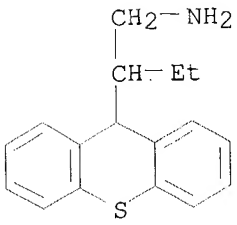
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



L10 ANSWER 31 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-88-0 REGISTRY
CN Thioxanthene-9-ethylamine, β-ethyl-, hydrochloride (8CI) (CA INDEX NAME)
MF C17 H19 N S . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)

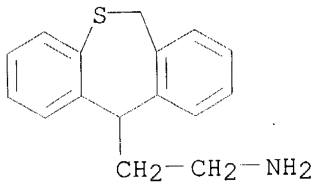


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:37664

L10 ANSWER 32 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-86-8 REGISTRY
CN Dibenzo[b,e]thiepin-11-ethylamine, 6,11-dihydro-, hydrochloride (8CI) (CA INDEX NAME)
MF C16 H17 N S . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)

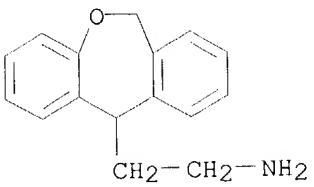


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:37664

L10 ANSWER 33 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-85-7 REGISTRY
CN Dibenz[b,e]oxepin-11-ethanamine, 6,11-dihydro- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Dibenz[b,e]oxepin-11-ethylamine, 6,11-dihydro- (8CI)
FS 3D CONCORD
MF C16 H17 N O
CI COM
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:107773

REFERENCE 2: 128:61341

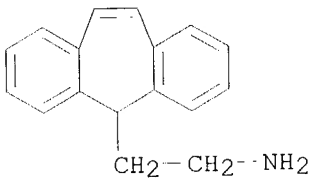
REFERENCE 3: 86:16562

REFERENCE 4: 82:156136

REFERENCE 5: 81:105324

REFERENCE 6: 70:37664

L10 ANSWER 34 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-84-6 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, hydrochloride (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5H-Dibenzo[a,d]cycloheptene-5-ethylamine, hydrochloride (8CI)
MF C17 H17 N . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation)
RL.NP Roles from non-patents: PREP (Preparation)
CRN (14451-09-3)



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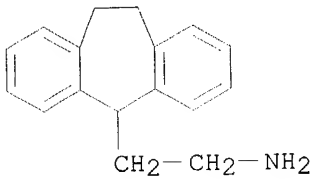
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 83:146868

REFERENCE 2: 70:37664

L10 ANSWER 35 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN

RN 21745-83-5 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro-, hydrochloride (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5H-Dibenzo[a,d]cycloheptene-5-ethylamine, 10,11-dihydro-, hydrochloride (8CI)
MF C17 H19 N . Cl H
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
CRN (21745-82-4)



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4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

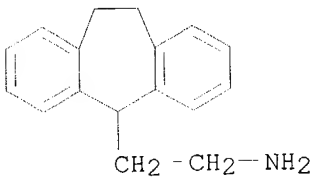
REFERENCE 1: 132:107773

REFERENCE 2: 132:93096

REFERENCE 3: 128:61341

REFERENCE 4: 70:37664

L10 ANSWER 36 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-82-4 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, 10,11-dihydro- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5H-Dibenzo[a,d]cycloheptene-5-ethylamine, 10,11-dihydro- (8CI)
FS 3D CONCORD
MF C17 H19 N
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:107773

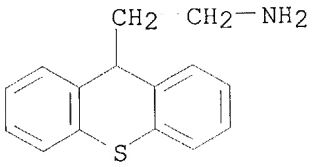
REFERENCE 2: 132:93096

REFERENCE 3: 130:66268

REFERENCE 4: 128:61341

REFERENCE 5: 70:37664

L10 ANSWER 37 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-81-3 REGISTRY
CN 9H-Thioxanthene-9-ethanamine (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Thioxanthene-9-ethylamine (8CI)
FS 3D CONCORD
MF C15 H15 N S
CI COM
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:160841

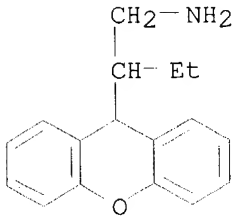
REFERENCE 2: 132:107773

REFERENCE 3: 130:66268

REFERENCE 4: 128:61341

REFERENCE 5: 70:37664

L10 ANSWER 38 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-78-8 REGISTRY
CN Xanthene-9-ethylamine, β-ethyl-, hydrochloride (8CI) (CA INDEX NAME)
MF C17 H19 N O . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)
CRN (686701-25-7)



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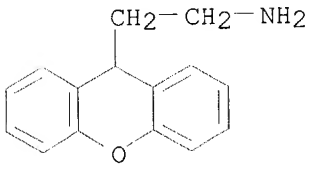
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:37664

L10 ANSWER 39 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-77-7 REGISTRY
CN 9H-Xanthene-9-ethanamine (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Xanthene-9-ethylamine (8CI)
FS 3D CONCORD
MF C15 H15 N O
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

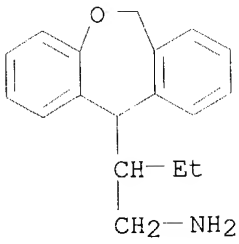
REFERENCE 1: 132:107773

REFERENCE 2: 130:66268

REFERENCE 3: 128:61341

L10 ANSWER 40 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21745-76-6 REGISTRY
CN Dibenz[b,e]oxepin-11-ethylamine, β-ethyl-6,11-dihydro-, hydrochloride (8CI) (CA INDEX NAME)
MF C18 H21 N O . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation)

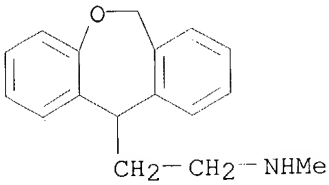


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:37664

L10 ANSWER 41 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21121-72-2 REGISTRY
CN Dibenz[b,e]oxepin-11-ethylamine, 6,11-dihydro-N-methyl-, hydrochloride (8CI) (CA INDEX NAME)
MF C17 H19 N O . Cl H
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)
CRN (55286-60-7)



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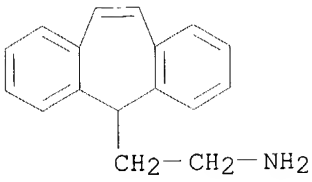
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:28839

L10 ANSWER 42 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 14451-09-3 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5H-Dibenzo[a,d]cycloheptene-5-ethylamine (8CI)
FS 3D CONCORD
MF C17 H17 N
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

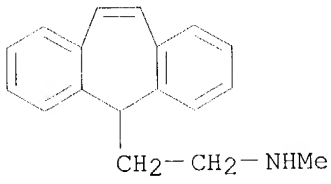
REFERENCE 1: 132:107773

REFERENCE 2: 130:66268

REFERENCE 3: 128:61341

REFERENCE 4: 83:146868

L10 ANSWER 43 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN
RN 7186-44-9 REGISTRY
CN 5H-Dibenzo[a,d]cycloheptene-5-ethanamine, N-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5H-Dibenzo[a,d]cycloheptene-5-ethylamine, N-methyl- (7CI)
FS 3D CONCORD
MF C18 H19 N
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

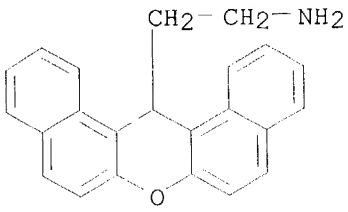
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 86:16562

REFERENCE 2: 65:65380

L10 ANSWER 44 OF 44 REGISTRY COPYRIGHT 2004 ACS on STN

RN 5768-67-2 REGISTRY
CN 14H-Dibenzo[a,j]xanthene-14-ethylamine (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H19 N O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 14:45:59 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 23 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 22 Jun 2004 (20040622/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L9	STR	
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L13	1394	SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L10
L14	300	SEA FILE=REGISTRY ABB=ON PLU=ON NMDA?
L15	23393	SEA FILE=HCAPLUS ABB=ON PLU=ON L14 OR NMDA?
L16	18792	SEA FILE=HCAPLUS ABB=ON PLU=ON L15(2A)RECEPTOR
L17	201	SEA FILE=HCAPLUS ABB=ON PLU=ON L13
L18	6	SEA FILE=HCAPLUS ABB=ON PLU=ON L17 AND L16
L19	6	SEA FILE=HCAPLUS ABB=ON PLU=ON L18 NOT L11

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=> d ibib abs hitrn l19 1-6

L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:158768 HCAPLUS
DOCUMENT NUMBER: 140:417748
TITLE: Serotonergic/glutamatergic interactions: the effects of mGlu2/3 receptor ligands in rats trained with LSD and PCP as discriminative stimuli
AUTHOR(S): Winter, J. C.; Eckler, J. R.; Rabin, R. A.
CORPORATE SOURCE: SUNY-Buffalo, Department of Pharmacology and Toxicology, School of Medicine and Biomedical Sciences, Buffalo, NY, 14214-3000, USA
SOURCE: Psychopharmacology (Berlin, Germany) (2004), 172(2), 233-240
CODEN: PSCHDL; ISSN: 0033-3158
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Rationale: On the basis of electrophysiol. evidence, it has been proposed that both antagonism of **NMDA receptors** by drugs such as PCP and stimulation of 5- HT2A receptors by drugs such as LSD result in the release of glutamate. Furthermore, it has been observed that antagonists and agonists at mGlu2/3 receptors increase and decrease, resp., the release of glutamate. Taken together, these observations predict behaviorally significant interactions between ligands at mGlu2/3 receptors and hallucinogens such as LSD and PCP. Objective: The present study sought to test in rats the glutamate hypothesis of hallucinogenesis using drug-induced stimulus control as the dependent variable and selected glutamatergic and serotonergic receptor ligands as independent variables. Methods: Male F-344 rats were trained in a two-lever, fixed ratio 10, food-reinforced task with either phencyclidine (PCP; 3.0 mg/kg; IP; 30 min pretreatment) or lysergic acid diethylamide (LSD; 0.1 mg/kg; IP; 15 min pretreatment) as discriminative stimuli. The interactions of PCP and the mGlu2/3 selective ligands, LY341495 and LY379268, with stimulus control by LSD were determined The effects of these drugs were compared with those of serotonergic antagonists known to antagonize the stimulus effects of LSD, specifically, pirenperone and M100907. Results: Stimulus control by LSD was potentiated by both PCP and the mGlu2/3 antagonist, LY341495. In tests of antagonism, stimulus control by LSD was significantly but incompletely diminished by the mGlu2/3 agonist, LY379268; this result was in contrast with the complete antagonism of LSD by both pirenperone and M100907. In PCP-trained rats, LY341495 was without effect on stimulus control by an intermediate dose of PCP. In contrast, the training dose of PCP was significantly but incompletely antagonized by LY379268. Conclusions: These data, obtained using a stimulus control model of the hallucinogenic effects of PCP and LSD, provide support for the hypothesis that glutamate release is a factor in hallucinogenesis by both 5-HT2 agonists and non-competitive NMDA antagonists.
IT **201943-63-7**, LY341495
RL: PAC (Pharmacological activity); BIOL (Biological study)
(serotonergic/glutamatergic interactions and the effects of mGlu2/3 receptor ligands in rats trained with LSD and PCP as discriminative stimuli)
REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:762261 HCAPLUS
DOCUMENT NUMBER: 138:50186

TITLE: Cardiovascular responses to activation of metabotropic glutamate receptors in the nTS of the rat
AUTHOR(S): Viard, Eddy; Sapru, Hreday N.
CORPORATE SOURCE: Department of Neurological Surgery, New Jersey Medical School, Newark, NJ, 07103-2757, USA
SOURCE: Brain Research (2002), 952(2), 308-321
CODEN: BRREAP; ISSN: 0006-8993
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Although several agonists and antagonists for different subtypes of metabotropic glutamate receptors (mGLURs) have become available in recent years, detailed information regarding their selectivity is not complete in the in vivo animal models. The purpose of the present investigation was to study the cardiovascular effects of microinjections of some of these mGLUR agonists and antagonists into the nucleus tractus solitarius (nTS). Microinjections (100 nl) of EC50 concns. of 3,5-DHPG (0.005 mM; mGLUR1 agonist), APDC (17.3 mM; mGLUR2/3 agonist), PPG (11.7 mM; mGLUR8 agonist) and L-AP4 (1 mM; mGLUR4 agonist) into the nucleus tractus solitarius of urethane-anesthetized male Wistar rats elicited depressor and bradycardic responses which may be mediated by pre- and/or postsynaptic mechanisms. The blocking effect of mGLUR antagonists used here was not specific for any one type of glutamate receptors (GLURs). For example, AIDA (50 mM; mGLUR1 antagonist) blocked the effects of EC50 concns. of 3,5-DHPG, and PPG. LY341495 (135 mM; mGLUR2/3 antagonist) blocked all of the mGLURs and ionotropic GLURs. EGLU, APICA and MCCG (250 mM each; mGLUR2/3 antagonists) blocked the effects of APDC, NMDA and AMPA. CPPG (80 mM) and MSOP (125 mM), mGLUR4 antagonists, blocked the effects of 3,5-DHPG, PPG and L-AP4. D-AP7 (**NMDA receptor** antagonist) and NBQX (a non-**NMDA receptor** antagonist) did not alter the responses of any of the mGLUR agonists. The data presented may be useful in assessing the role of metabotropic and ionotropic GLURs in mediating different cardiovascular reflexes.

IT **201943-63-7**, LY341495
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(cardiovascular responses to activation of metabotropic glutamate receptors in nucleus tractus solitarius by excitatory amino acid receptor agonists and antagonists)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:735784 HCAPLUS
DOCUMENT NUMBER: 133:344557
TITLE: A novel, competitive mGlu5 receptor antagonist (LY344545) blocks DHPG-induced potentiation of NMDA responses but not the induction of LTP in rat hippocampal slices
AUTHOR(S): Doherty, A. J.; Palmer, M. J.; Bortolotto, Z. A.; Hargreaves, A.; Kingston, A. E.; Ornstein, P. L.; Schoepp, D. D.; Lodge, D.; Collingridge, G. L.
CORPORATE SOURCE: MRC Centre for Synaptic Plasticity, Department of Anatomy, School of Medical Sciences, University of Bristol, Bristol, BS8 1TD, UK
SOURCE: British Journal of Pharmacology (2000), 131(2), 239-244
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors have investigated the pharmacol. properties of LY344545, a structurally related epimer of the broad spectrum competitive metabotropic glutamate receptor antagonist, LY341495. The authors have found that

LY344545 also antagonizes competitively nearly all mGlu receptor subtypes, but with a wide spectrum of activity. The order of potency for the human receptor isoforms was mGlu5a (IC50 of 5.5±0.6 μM)>mGlu2=mGlu3>mGlu1α=mGlu7>mGlu6=mGlu8. No significant mGlu4 receptor antagonist activity was detected at the highest concentration used (100 μM). 100 μM LY344545 displaced 50±5% of [3H]-CGP39653 binding, but less than 30% of [3H]-kainate or [3H]-AMPA in radioligand binding assays. LY344545 antagonized L-glutamate stimulated Ca2+ release in CHO cells transfected with mGlu receptors in a concentration dependent manner with a 10-fold higher affinity for the rat mGlu5a receptor (Ki=2.1±0.6 μM) compared to the rat mGlu1α receptor (Ki=20.5±2.1 μM). 50 μM (1S, 3R)-ACPD-induced Ca2+ rises in hippocampal CA1 neurons were also antagonized (IC50=6.8±0.7 μM). LY344545 antagonized 10 μM (S)-3,5-DHPG-induced potentiation of NMDA depolarizations in CA1 neurons (EC50=10.6±1.0 μM). At higher concns. (≥100 μM), LY344545 was an **NMDA receptor** antagonist. LY344545 also blocked the induction, but not the expression, of LTP at CA3 to CA1 synapses with an IC50>300 μM. This effect is consistent with its weak activity at **NMDA receptors**. These results demonstrate that the binding of ligands to mGlu receptor subtypes is critically dependent on the spatial orientation of the same mol. substituents within a given chemical pharmacophore. The identification of LY344545 as the first competitive antagonist to show selectivity towards mGlu5 receptors supports the potential to design more selective and potent competitive antagonists of this receptor. These results further indicate that mGlu receptor-mediated potentiation of NMDA responses is not essential for the induction of LTP.

IT **201851-20-9**, LY 344545
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(novel competitive mGlu5 receptor antagonist LY344545 blocks DHPG-induced potentiation of NMDA responses but not induction of LTP in rat hippocampal slices)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:74530 HCAPLUS
DOCUMENT NUMBER: 132:217391
TITLE: Neuroprotective actions of novel and potent ligands of group I and group II metabotropic glutamate receptors
AUTHOR(S): Kingston, A. E.; O'Neill, M. J.; Bond, A.; Bruno, V.; Battaglia, G.; Nicoletti, F.; Harris, J. R.; Clark, B. P.; Monn, J. A.; Lodge, D.; Schoepp, D. D.
CORPORATE SOURCE: Eli Lilly and Co. Ltd., Windlesham, Surrey, GU20 6PH, UK
SOURCE: Annals of the New York Academy of Sciences (1999), 890(Neuroprotective Agents), 438-449
CODEN: ANYAA9; ISSN: 0077-8923
PUBLISHER: New York Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The role of group I metabotropic glutamate (mGlu) receptors in neurodegeneration is controversial because of the contradictory effects of mGlu1/5 agonists in in vitro models of neuronal cell death. In this study, novel and selective antagonists of mGlu1 and mGlu5: LY367385 and LY367366 were found to show consistent neuroprotective effects against N-methyl-D-aspartate (NMDA)-induced excitotoxicity in vitro and in vivo. Furthermore, intraventricular administration of LY367385 reduced hippocampal cell death in gerbils subjected to transient global ischemia. Previous studies have also shown that activation of group II mGlu receptors may contribute to neuroprotective mechanisms in vitro and in vivo. Three potent group II mGlu agonists-LY354740, LY379268 and

LY389795-were found to attenuate both NMDA excitotoxicity and staurosporine-induced neuronal cell death. LY354740 and LY379268 were protective against transient global ischemia in gerbils when dosed i.p. These results support the view that antagonists of mGlu1 and mGlu5 and agonists of group II mGlu receptors may be useful agents in the therapeutic treatment of neurodegenerative disease.

IT **209332-61-6**, LY367366
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(neuroprotective actions of novel and potent ligands of group I and group II metabotropic glutamate receptors)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:581440 HCAPLUS
DOCUMENT NUMBER: 132:18696
TITLE: DHPG-induced LTD in area CA1 of juvenile rat hippocampus; characterization and sensitivity to novel mGlu receptor antagonists
AUTHOR(S): Fitzjohn, S. M.; Kingston, A. E.; Lodge, D.; Collingridge, G. L.
CORPORATE SOURCE: MRC Centre for Synaptic Plasticity, School of Medical Sciences, Department of Anatomy, University of Bristol, Bristol, UK
SOURCE: Neuropharmacology (1999), 38(10), 1577-1583
CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have used extracellular microelectrode recording to characterize a form of long-term depression (LTD) of synaptic transmission that can be induced by metabotropic glutamate (mGlu) receptor activation in the CA1 region of the young (12-18 day old) rat hippocampus. Activation of group I mGlu receptors by the specific agonist 3,5-dihydroxyphenylglyine (DHPG) induced LTD of field excitatory postsynaptic potentials (fEPSPs). The mGlu5 selective agonist 2-chloro-5-hydroxyphenylglycine was also capable of inducing LTD. In contrast, the group II specific agonist DCG-IV had no effect on synaptic transmission, while the group III receptor agonist (S)-2-amino-4-phosphonobutyrate elicited a depression that reversed fully upon agonist washout. DHPG-induced LTD could still be generated after prior saturation of elec.-induced **NMDA receptor**-dependent LTD. DHPG-induced LTD was reversed by tetanic stimulation comprising 100 shocks delivered at 100 Hz. A novel mGlu receptor antagonist, (RS)-2-amino-2-(3-cis and trans-carboxycyclobutyl-3-(9-thioxanthyl)propionic acid) (LY393053) that potently inhibits mGlu1 and mGlu5 receptors, prevented the induction of DHPG-induced LTD. Like other mGlu receptor antagonists, LY393053 also reversed pre-established DHPG-induced LTD. In contrast, a potent mGlu1 selective antagonist (S)-2-methyl-4-carboxyphenylglycine (LY367385) did not prevent the induction of DHPG-induced LTD. In conclusion, DHPG, probably via activation of mGlu5 receptors, is able to induce a robust form of LTD in the CA1 region of the young rat hippocampus that is mechanistically distinct from **NMDA receptor**-dependent homosynaptic LTD.

IT **206444-72-6**, LY 393053
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(DHPG-induced long-term depression in area CA1 of juvenile rat hippocampus; characterization and sensitivity to novel mGlu receptor antagonists)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:25332 HCAPLUS
DOCUMENT NUMBER: 130:177834
TITLE: The potent mGlu receptor antagonist LY341495 identifies roles for both cloned and novel mGlu receptors in hippocampal synaptic plasticity
AUTHOR(S): Fitzjohn, S. M.; Bortolotto, Z. A.; Palmer, M. J.; Doherty, A. J.; Ornstein, P. L.; Schoepp, D. D.; Kingston, A. E.; Lodge, D.; Collingridge, G. L.
CORPORATE SOURCE: Department of Anatomy, University of Bristol, Bristol, BS8 ITD, UK
SOURCE: Neuropharmacology (1998), 37(12), 1445-1458
CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Understanding the roles of metabotropic glutamate (mGlu) receptors has been severely hampered by the lack of potent antagonists. LY341495 (2S-2-amino-2-(1S,2S-2-carboxycyclopropyl-1-yl)-3-(xanth-9-yl)propanoic acid) has been shown to block group II mGlu receptors in low nanomolar concns. (Kingston, A.E., Ornstein, P.L., Wright, R.A., Johnson, B.G., Mayne, N.G., Burnett, J.P., Belagaje, R., Wu, S., Schoepp, D.D., 1998. LY341495 is a nanomolar potent and selective antagonist at group II metabotropic glutamate receptors. Neuropharmacol. 37, 1-12) but can be used in higher concns. to block all hippocampal mGlu receptors, identified so far by mol. cloning (mGlu1-5, 7,8). Here we have further characterized the mGlu receptor antagonist activity of LY341495 and have used this compound to investigate roles of mGlu receptors in hippocampal long-term potentiation (LTP) and long-term depression (LTD). LY341495 competitively antagonized DHPG-stimulated PI hydrolysis in AV12-664 cells expressing either human mGlu1 or mGlu5 receptors with Ki-values of 7.0 and 7.6 μM, resp. When tested against 10 μM L-glutamate-stimulated Ca2+ mobilization in rat mGlu5 expressing CHO cells, it produced substantial or complete block at a concentration of 100 μM. In rat hippocampal slices, LY341495 eliminated 30 μM DHPG-stimulated PI hydrolysis and 100 μM (1S,3R)-ACPD-inhibition of forskolin-stimulated cAMP formation at concns. of 100 and 0.03 μM, resp. In area CA1, it antagonized DHPG-mediated potentiation of NMDA-induced depolarizations and DHPG-induced long-lasting depression of AMPA receptor-mediated synaptic transmission. LY341495 also blocked **NMDA receptor**-independent depotentiation and setting of a mol. switch involved in the induction of LTP; effects which have previously been shown to be blocked by the mGlu receptor antagonist (S)-MCPG. These effects may therefore be due to activation of cloned mGlu receptors. In contrast, LY341495 did not affect **NMDA receptor**-dependent homosynaptic LTD; an effect which may therefore be independent of cloned mGlu receptors. Finally, LY341495 failed to antagonize **NMDA receptor**-dependent LTP and, in area CA3, **NMDA receptor**-independent, mossy fiber LTP. Since in the same inputs these forms of LTP were blocked by (S)-MCPG, a novel type of mGlu receptor may be involved in their induction.

IT **201943-63-7**, LY341495
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(mGlu receptor antagonist LY341495 identifies roles for both cloned and novel mGlu receptors in hippocampal synaptic plasticity)

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L14          300 SEA FILE=REGISTRY ABB=ON  PLU=ON  NMDA?
L15        23393 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L14 OR NMDA?
L16        18792 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15(2A)RECEPTOR
L17          201 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L13
L18            6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L16
L19            6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 NOT L11
L20            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L15 AND L17) NOT (L11 OR
                 L19)


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L20  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1999:581433  HCAPLUS
DOCUMENT NUMBER:          131:346906
TITLE:                    Evaluation of agonists and antagonists acting at Group
                          I metabotropic glutamate receptors in the thalamus in
                          vivo
AUTHOR(S):                Salt, T. E.; Turner, J. P.; Kingston, A. E.
CORPORATE SOURCE:         Institute of Ophthalmology, University College London,
                          London, UK
SOURCE:                   Neuropharmacology (1999), 38(10), 1505-1510
                          CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER:                Elsevier Science Ltd.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Recordings were made from single neurons in the ventrobasal thalamus of
     anesthetized rats in order to evaluate the properties of several agonists
     and antagonists of Group I mGlu receptors.  The selective mGlu1 receptor
     antagonist LY 367385 was found to reduce excitatory responses to
     iontophoretically applied ACPD and DHPG whereas the mGlu5 agonist CHPG was
     resistant to antagonism.  The antagonists LY 367366 and LY 393053 reduced
     responses to all three agonists, but without reducing responses to
     NMDA or AMPA.  Although AIDA was also found to reduce mGlu
     agonist-evoked responses, this antagonist also produced significant redns.
     in responses to NMDA and AMPA.  These data suggest that there
     are functional mGlu1 and mGlu5 receptors in the thalamus.  Furthermore, LY
     367385 is a useful tool for investigating mGlu1 functions whereas LY
     367366 and LY 393053 have a broader spectrum of action.  The usefulness of
     AIDA as an antagonist in physiol. expts. would appear to be limited by its
     effects against NMDA and AMPA.
IT   6384-92-5, NMDA
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); BIOL (Biological study)
        (group I metabotropic glutamate receptor agonist and antagonist
        evaluation in the thalamus in vivo)
IT   206444-72-6, LY 393053 209332-61-6, LY 367366
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); BUU (Biological use, unclassified); BIOL (Biological
     study); USES (Uses)
        (group I metabotropic glutamate receptor agonist and antagonist
        evaluation in the thalamus in vivo)
REFERENCE COUNT:          22    THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
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RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:187940 HCAPLUS
DOCUMENT NUMBER: 130:332754
TITLE: Neuroprotective activity of the potent and selective mGlu1a metabotropic glutamate receptor antagonist, (+)-2-methyl-4-carboxyphenylglycine (LY367385): comparison with LY357366, a broader spectrum antagonist with equal affinity for mGlu1a and mGlu5 receptors
AUTHOR(S): Bruno, V.; Battaglia, G.; Kingston, A.; O'Neill, M. J.; Catania, M. V.; Di Grezia, R.; Nicoletti, F.
CORPORATE SOURCE: I.N.M. Neuromed, Pozzilli, Italy
SOURCE: Neuropharmacology (1999), 38(2), 199-207
CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB (+)-2-Methyl-4-carboxyphenylglycine (LY367385), a potent and selective antagonist of mGlu1a metabotropic glutamate receptors, was neuroprotective in the following in vitro and in vivo models of excitotoxic death: (i) mixed cultures of murine cortical cells transiently exposed to N-methyl-D-aspartate (**NMDA**); (ii) rats monolaterally infused with **NMDA** into the caudate nucleus; and (iii) gerbils subjected to transient global ischemia. The authors have compared the activity of LY367385 with that of the novel compound (±)-α-thioxanthylmethyl-4-carboxyphenylglycine (LY367366), which antagonizes both mGlu1a and -5 receptors at low micromolar concns., but also recruits other subtypes at higher concns. Although LY367366 was neuroprotective, it was in general less efficacious than LY357385, suggesting that inhibition of mGlu1 receptors is sufficient to confer significant neuroprotection. The authors conclude that endogenous activation of mGlu1a receptor (or perhaps other mGlu1 receptors splice variants) contributes to the development of neuronal degeneration of excitotoxic origin.
IT **6384-92-5**, **NMDA**
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(excitotoxin; neuroprotective activity of mGlu1a metabotropic glutamate receptor antagonist LY367385 in comparison with LY357366 in excitotoxic death models)
IT **209332-61-6**, LY 367366
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(neuroprotective activity of mGlu1a metabotropic glutamate receptor antagonist LY367385 in comparison with LY357366 in excitotoxic death models)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:763175 HCAPLUS
DOCUMENT NUMBER: 130:105594
TITLE: Characterization of (2S,2'R,3'R)-2-(2',3'-[3H]-Dicarboxycyclopropyl)glycine binding in rat brain
AUTHOR(S): Mutel, Vincent; Adam, Geo; Chaboz, Sylvie; Kemp, John A.; Klingelschmidt, Agnes; Messer, Jurg; Wichmann, Jurgen; Woltering, Thomas; Richards, John Grayson
CORPORATE SOURCE: Pharma Division Preclinical CNS Research, F. Hoffmann-La Roche Ltd., Basel, CH-4070, Switz.
SOURCE: Journal of Neurochemistry (1998), 71(6), 2558-2564
CODEN: JONRA9; ISSN: 0022-3042

PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB (2S,2'R,3'R)-2-(2',3'-[3H]Dicarboxycyclopropyl)glycine ([3H]DCG IV) binding was characterized in vitro in rat brain cortex homogenates and rat brain sections. In cortex homogenates, the binding was saturable and the saturation isotherm indicated the presence of a single binding site with a KD value of 180 nM and a Bmax of 780 fmol/mg of protein. The nonspecific binding, measured using 100 μM LY 354740, was <30%. **NMDA**, AMPA, kainate, L(-)-threo-3-hydroxyaspartic acid, and (S)-3,5-dihydroxyphenylglycine were all inactive in [3H]DCG IV binding up to 1 mM. However, several compds. inhibited [3H]DCG IV binding in a concentration-dependent manner with the following rank order of potency: LY 341495 = LY 354740 > DCG IV = (2S,1'S,2'S)-2-(2-carboxycyclopropyl)glycine > (1S,3R)-1-amino-cyclopentane-1,3-dicarboxylic acid > (2S,1'S,2'S)-2-methyl-2-(2-carboxycyclopropyl)glycine > L-glutamate = ibotenate > quisqualate > (RS)-α-methyl-4-phosphonophenylglycine = L(+)-2-amino-3-phosphonopropionic acid > (S)-α-methyl-4-carboxyphenylglycine > (2S)-α-ethylglutamic acid > L(+)-2-amino-4-phosphonobutyric acid. N-Acetyl-L-aspartyl-L-glutamic acid inhibited the binding in a biphasic manner with an IC50 of 0.2 μM for the high-affinity component. The binding was also affected by GTPγS, reducing agents, and CdCl2. In parasagittal sections of rat brain, a high d. of specific binding was observed in the accessory olfactory bulb, cortical regions (layers 1, 3, and 4 > 2, 5, and 6), caudate putamen, mol. layers of the hippocampus and dentate gyrus, subiculum, presubiculum, retrosplenial cortex, anteroventral thalamic nuclei, and cerebellar granular layer, reflecting its preferential (perhaps not exclusive) affinity for pre- and postsynaptic metabotropic glutamate mGlu2 receptors. Thus, the pharmacol., tissue distribution, and sensitivity to GTPγS show that [3H]DCG IV binding is probably to group II metabotropic glutamate receptors in rat brain.
IT **201943-63-7**, LY 341495
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
((dicarboxycyclopropyl)glycine binding in rat brain and regional and pharmacol. characterization thereof)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> => select hit rn l19 1-6
E1 THROUGH E4 ASSIGNED

=> select hit rn l20 1-3
E5 THROUGH E8 ASSIGNED

=> fil reg
FILE 'REGISTRY' ENTERED AT 14:47:33 ON 23 JUN 2004
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7
DICTIONARY FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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=>

=> => s e1-e8 and l5
1 201943-63-7/BI
(201943-63-7/RN)
1 201851-20-9/BI
(201851-20-9/RN)
1 206444-72-6/BI
(206444-72-6/RN)
1 209332-61-6/BI
(209332-61-6/RN)
1 209332-61-6/BI
(209332-61-6/RN)
1 6384-92-5/BI
(6384-92-5/RN)
1 201943-63-7/BI
(201943-63-7/RN)
1 206444-72-6/BI
(206444-72-6/RN)
L21 4 (201943-63-7/BI OR 201851-20-9/BI OR 206444-72-6/BI OR 209332-61-6/BI OR 209332-61-6/BI OR 6384-92-5/BI OR 201943-63-7/BI OR 206444-72-6/BI) AND L5

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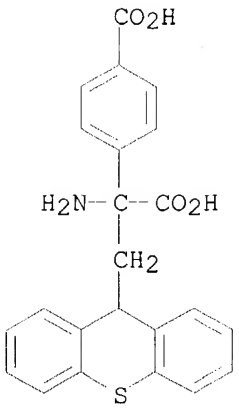
L21 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN
RN **209332-61-6** REGISTRY
CN 9H-Thioxanthene-9-propanoic acid, α-amino-α-(4-carboxyphenyl)-
(9CI) (CA INDEX NAME)
OTHER NAMES:
CN LY 367366
FS 3D CONCORD
MF C23 H19 N O4 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, EMBASE, PROUSDDR, SYNTHLINE, TOXCENTER, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)
10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:358926

REFERENCE 2: 138:379002

REFERENCE 3: 138:198858

REFERENCE 4: 138:130580

REFERENCE 5: 137:241510

REFERENCE 6: 136:177837

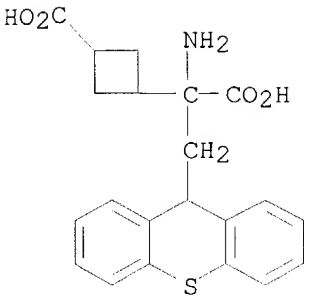
REFERENCE 7: 132:217391

REFERENCE 8: 131:346906

REFERENCE 9: 130:332754

REFERENCE 10: 129:81968

L21 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN
RN **206444-72-6** REGISTRY
CN 9H-Thioxanthene-9-propanoic acid, α-amino-α-(3-carboxycyclobutyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN LY 393053
FS 3D CONCORD
MF C21 H21 N O4 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, EMBASE, PROUSDDR, SYNTHLINE, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:379002

REFERENCE 2: 136:241521

REFERENCE 3: 132:202986

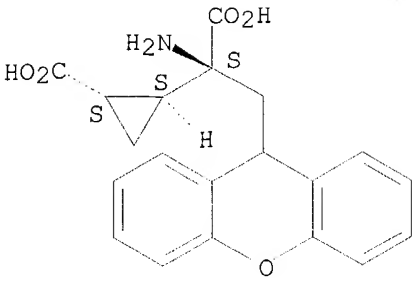
REFERENCE 4: 132:18696

REFERENCE 5: 131:346906

REFERENCE 6: 128:308743

L21 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN
RN **201943-63-7** REGISTRY
CN 9H-Xanthene-9-propanoic acid, α-amino-α-[(1S,2S)-2-carboxycyclopropyl]-, (αS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9H-Xanthene-9-propanoic acid, α-amino-α-(2-carboxycyclopropyl)-, [1S-[1α(R*),2β]]-
OTHER NAMES:
CN LY 341495
FS STEREOSEARCH
MF C20 H19 N O5
SR CA
LC STN Files: BIOSIS, BIOTECHNO, CA, CAPLUS, CHEMCATS, CSCHEM, EMBASE, IMSDRUGNEWS, IMSRESEARCH, PHAR, PROUSDDR, SYNTHLINE, TOXCENTER, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

33 REFERENCES IN FILE CA (1907 TO DATE)
33 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:417748

REFERENCE 2: 140:350413

REFERENCE 3: 140:332336

REFERENCE 4: 140:314919

REFERENCE 5: 140:264522

REFERENCE 6: 140:229199

REFERENCE 7: 140:192778

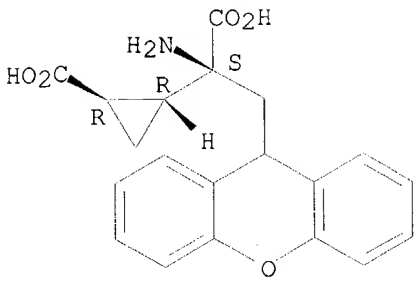
REFERENCE 8: 140:70874

REFERENCE 9: 139:270878

REFERENCE 10: 139:160362

L21 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2004 ACS on STN
RN **201851-20-9** REGISTRY
CN 9H-Xanthene-9-propanoic acid, α-amino-α-[(1R,2R)-2-carboxycyclopropyl]-, (αS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 9H-Xanthene-9-propanoic acid, α-amino-α-(2-carboxycyclopropyl)-, [1R-[1α(S*),2β]]-
OTHER NAMES:
CN LY 344545
FS STEREOSEARCH
MF C20 H19 N O5
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, PROUSDDR, SYNTHLINE, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:344557

REFERENCE 2: 128:180675

REFERENCE 3: 128:123439

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